

Adaptive Smoothing of the Log-Spectrum with Multiple Tapering *

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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-multiple taper estimate. This procedure reduces the expected mean square error by $(\frac{\pi^2}{4})^{4/5}$ over simply smoothing the log tapered periodogram. A data adaptive implementation of a variable bandwidth kernel smoother is given.

1 INTRODUCTION

We consider a discrete, stationary, Gaussian time series $\{x_j, j = 1, \dots, N\}$ with a smooth spectral density, $S(f)$, which is bounded away from zero. The autocovariance is the Fourier transform of the spectral density: $\text{Cov}[x_j, x_k] = \int_{-\frac{1}{2}}^{\frac{1}{2}} S(f) e^{2\pi i(j-k)f} df$. When the logarithm of the spectral density, $\theta(f) \equiv \ln[S(f)]$, is desired, two common approaches are: 1) to estimate the spectral density and then transform to the logarithm; and 2) to smooth the logarithm of the tapered periodogram. The first approach can be sensitive to broad-band bias when the spectral range is large, while the second approach inflates the variance of the estimate [7, Ch. 6.15], [14]. We propose a combined estimator of the log-spectral density with the robustness properties of the second estimator without its variance inflation.

In Section 2, we consider quadratic estimates of the spectral density. In Section 3, we consider kernel smoothing the multi-taper spectral estimate. In Section 4, the logarithm of

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the multi-taper spectral estimate is kernel smoothed to estimate the log-spectral density. In Section 5, we consider a data adaptive variable bandwidth implementation of this method. In Section 6, we present our simulation results. Sections 7 and 8 discuss and summarize our results. In the appendix, we describe a new method for selecting the initial halfwidth.

2 STATISTICS OF MULTI-TAPER SPECTRAL ESTIMATORS

Every quadratic, modulation-invariant spectral estimator has the form

$$\hat{S}_{mt}(f) = \sum_{m,n=1}^N q_{mn} x_m x_n e^{2\pi i(m-n)f}, \quad (1)$$

where $\mathbf{Q} = [q_{mn}]$ is a self-adjoint matrix [2, 5]. Decomposing \mathbf{Q} into its eigenvector representation, $\mathbf{Q} = \sum_{k=1}^K \mu_k \boldsymbol{\nu}^{(k)} \boldsymbol{\nu}^{(k)\dagger}$, (1) can be recast as

$$\hat{S}_{mt}(f) = \sum_{k=1}^K \mu_k \left| \sum_{n=1}^N \nu_n^{(k)} x_n e^{-2\pi i n f} \right|^2, \quad (2)$$

where the $\boldsymbol{\nu}^{(k)}$ are the orthonormal eigenvectors of \mathbf{Q} and the μ_k are the eigenvalues. We call (2) the multiple taper representation of the spectral estimate [7, 10, 13]. (This name is often shortened to multi-taper and sometimes referred to as a multiple spectral window estimate.) In practice, quadratic spectral estimators are constructed by specifying the eigenvectors/tapers and the weights. For concreteness, we will usually use the sinusoidal tapers $\nu_m^{(k)} = \sqrt{\frac{2}{N+1}} \sin\left(\frac{\pi k m}{N+1}\right)$ [12]. For these tapers, the spectral estimate (2) can be recast as

$$\hat{S}_{mt}(f) = \Delta \sum_{k=1}^K \mu_k |\zeta(f+k\Delta) - \zeta(f-k\Delta)|^2, \quad (3)$$

where $\Delta = \frac{1}{2N+2}$ and $\zeta(f)$ is the discrete Fourier transform of $\{x\}$: $\zeta(f) = \sum_{n=1}^N x_n e^{-2\pi i n f}$. The corresponding smoothed periodogram estimate, $\hat{S}_{sp}(f) = \sum_{k=-K}^K |\zeta(f+k\Delta)|^2 / (2KN + N)$, has an appreciably larger bias. The sinusoidal multi-taper estimate reduces the bias since the sidelobes of $\zeta(f+k\Delta)$ are partially cancelled by those of $\zeta(f-k\Delta)$.

To analyze the multi-taper estimate, we use the local white noise approximation [3], which corresponds to assuming that the combined estimator of $\theta(f)$ has its domain of dependence concentrated near frequency f . When $\mu_k = 1/K$, $\hat{S}_{mt}(f)/S(f)$ has a $\chi_{2K}^2/(2K)$ distribution to leading order in K/N [14]. Note $\mathbf{E}[\ln(\chi_{2K}^2/(2K))] = \psi(K) - \ln(K)$, $\mathbf{Var}[\ln(\chi_{2K}^2/(2K))] = \psi'(K)$, where ψ is the digamma function and ψ' is the trigamma function. The multi-taper estimate of the logarithm of the spectral density is

$$\hat{\theta}_{mt}(f) \equiv \ln[\hat{S}_{mt}(f)] - [\psi(K) - \ln(K)]. \quad (4)$$

An alternative estimate of $\ln[S(f)]$ is to average the logarithms of the individual multi-taper estimates:

$$\overline{\ln[\hat{S}_{st}(f)]} \equiv \frac{1}{K} \sum_{k=1}^K \ln\left(\frac{|\zeta(f+k\Delta) - \zeta(f-k\Delta)|^2}{2(N+1)}\right), \quad (5)$$

where the subscript ‘‘st’’ denotes single taper. Since the χ_2^2 distribution has its most probable value at zero, the distribution of its logarithm has a very long lower tail. This lower tail induces bias and increases the variance in the estimate: $\mathbf{Bias}[\ln(\hat{S}_{st})] \simeq -0.577$, and $\mathbf{Var}[\ln(\hat{S}_{st})] = \psi'(1)/K = \pi^2/(6K)$. By averaging the K estimates prior to taking the logarithm, we reduce both the bias and the variance. The variance reduction factor if one averages and then takes logarithms, $\ln[\hat{S}(f)]$, is $K\psi'(K)/\psi'(1)$. For large K , $K\psi'(K) \simeq 1 + \frac{1}{2K}$, so the variance reduction factor (of reversing the order of the operations in (5)) is asymptotically $6/\pi^2$.

The local bias of the multi-taper estimate is

$$\mathbf{E}[\hat{S}_{mt}(f) - S(f)] \simeq \frac{S''(f)}{2} \sum_{k=1}^K \mu_k \int_{-\frac{1}{2}}^{\frac{1}{2}} |f'|^2 |V^{(k)}(f')|^2 df', \quad (6)$$

where the k -th spectral window, $V^{(k)}$, is the Fourier transform of the k -th taper, $\nu^{(k)}$: $V^{(k)}(f) = \sum_{n=1}^N \nu_n^{(k)} e^{-2\pi inf}$. Equation (6) neglects the nonlocal bias and assumes $\sum_{k=1}^K \mu_k = 1$. For the sinusoidal tapers with uniform weighting ($\mu_k = 1/K$), (6) reduces to

$$\mathbf{Bias}[\hat{S}_{mt}(f)] \simeq \frac{S''(f)}{8} \sum_{k=1}^K \mu_k \frac{k^2}{N^2} = S''(f) \frac{K^2}{24N^2}, \quad (7)$$

where the intermediate equality is derived in [12]. Noting that $S''(f)/S(f) = [\theta''(f) + |\theta'(f)|^2]$, the local bias of the estimate (4) for the uniformly weighted sinusoidal tapers is

$$\mathbf{E}[\hat{\theta}_{mt}(f) - \theta(f)] \simeq [\theta''(f) + |\theta'(f)|^2] \frac{K^2}{24N^2}. \quad (8)$$

3 SMOOTHED MULTI-TAPER ESTIMATE

We now consider kernel estimators of $\partial_f^q S(f)$ which smooth the multi-taper estimate:

$$\widehat{\partial_f^q S_\kappa}(f) \equiv \frac{1}{h^{q+1}} \int_{-\frac{1}{2}}^{\frac{1}{2}} \kappa\left(\frac{f' - f}{h}\right) \hat{S}_{mt}(f') df', \quad (9)$$

where the $\hat{\cdot}$ over $\partial_f^q S_\kappa$ denotes the estimate of the q th derivative. The subscript on \hat{S}_κ denotes the two-stage estimator constructed by first multi-tapering and then kernel smoothing. Here $\kappa(f)$ is a kernel with Lipschitz smoothness of degree 2 with support in $[-1, 1]$, and $\kappa(\pm 1) = 0$. The bandwidth parameter is h . We say a kernel is of order (q, p) if $\int f^m \kappa(f) df =$

$m! \delta_{m,q}$, $m = 0, \dots, p-1$. We denote the p th moment of a kernel of order (q, p) by $B_p \equiv \int f^p \kappa(f) df / p!$. For function estimation ($q = 0$), we use $p = 2$ and $p = 4$. To estimate the second derivative, we use a kernel of order $(2, 4)$.

Smoothing the multi-taper estimate replaces the original quadratic estimator in (1) by another quadratic estimator, $\tilde{\mathbf{Q}}$ with $\tilde{Q}_{mn} = \hat{\kappa}_{m-n} \sum_{k=1}^K \mu_k \nu_m^{(k)} \nu_n^{(k)}$, where $\hat{\kappa}_m$ is the Fourier transform of the kernel smoother: $\hat{\kappa}_m \equiv h^{-(q+1)} \int \kappa(\frac{f'}{h}) e^{imf'} df'$. By Theorem 5.2 of Riedel & Sidorenko [12], this smoothed multi-taper estimator cannot outperform the pure multi-taper method with minimum bias tapers.

Theorem 3.1 *Let $S(f)$ be twice continuously differentiable with $0 < S_{\min} \leq S(f) \leq S_{\max} < \infty$. Consider the kernel smoothed multi-tapered spectral estimate (9) with K tapers. Let the kernel, $\kappa(f)$, be of order (q, p) and have Lipschitz smoothness of degree 2. Let the envelope of the spectral windows, $V^{(k)}(f)$, decay as $(Nf)^{-1}$ or faster for $f > K/N$ and assume that $\nu_{n+m}^{(k)} \simeq \nu_n^{(k)} [1 + \mathcal{O}(\frac{Km}{N})]$. Consider the limit that $N \rightarrow \infty$, $h \rightarrow 0$ and $K \rightarrow \infty$, such that $K/(Nh) \rightarrow 0$. The kernel smoothed multi-tapered estimate (9) has asymptotic variance:*

$$\mathbf{Var} \left[\widehat{\partial_f^q S_\kappa(f)} \right] \simeq \frac{\|\kappa\|^2 S(f)^2}{h^{2q+1}} \sum_{k,k'=1}^K \mu_k \mu_{k'} \left(\sum_{n=1}^N |\nu_n^{(k)}|^2 |\nu_n^{(k')}|^2 \right) + \mathcal{O}_{\mathcal{R}} \left(\left(\frac{K}{Nh} \right)^{4/5} + \left(\frac{h}{K} \right)^2 \right), \quad (10)$$

where $\|\kappa\|^2 \equiv \int_{-1}^1 \kappa(f)^2 df$.

We use the notation $\mathcal{O}_{\mathcal{R}}(\cdot)$ to denote a size of $\mathcal{O}(\cdot)$ relative to the main term. The condition, $\frac{K}{N}/h \rightarrow 0$, implies that the smoothing from multi-tapering is much less than the smoothing from kernel averaging. The condition that $\nu_{n+m}^{(k)} \simeq \nu_n^{(k)} [1 + \mathcal{O}(\frac{Km}{N})]$ is fulfilled when the k -th taper has a scale length of variation of N/k . The sinusoidal tapers satisfy this condition as do the Slepian tapers when their bandwidth parameter, W , is chosen as K/N .

Proof: We separate the variance into a broad-banded contribution $\approx 1/(N|f - f'|)^2$ for $|f - f'| \gg K/Nh$ and a local contribution $\approx |f - f'|^2$. The broad-band contribution is $\mathcal{O}_{\mathcal{R}}((\frac{hN}{KN})^2)$. The local contribution differs from a locally white process by $\mathcal{O}_{\mathcal{R}}(S''(f)^2 (\frac{K}{2Nh})^2)$. We now consider the local contribution in the locally white noise approximation [3]. Using the Gaussian fourth moment identity and resummation yields

$$\mathbf{Var} \left[\widehat{\partial_f^q S_\kappa(f)} \right] \simeq S(f)^2 \text{tr}[\tilde{\mathbf{Q}}\tilde{\mathbf{Q}}] = S(f)^2 \sum_{k,k'=1}^K \mu_k \mu_{k'} \sum_{n=1}^N \sum_{m=1-n}^{N-n} \hat{\kappa}_m^2 \nu_{n+m}^{(k)} \nu_n^{(k)} \nu_{n+m}^{(k')} \nu_n^{(k')}. \quad (11)$$

Our kernel, $\kappa(\cdot)$ is Lipschitz of degree 2, and therefore $\hat{\kappa}_m \sim \mathcal{O}(\|\hat{\kappa}\|/(mh)^2)$ for $mh \gg 1$. Expanding $\nu_{n+m}^{(k)}$ in mK/N and truncating in m yields

$$\mathbf{Var} \left[\widehat{\partial_f^q S_\kappa(f)} \right] \simeq S(f)^2 \sum_{k,k'=1}^K \mu_k \mu_{k'} \left(\sum_{n=1}^N |\nu_n^{(k)}|^2 |\nu_n^{(k')}|^2 \right) \left(\sum_{m=1}^N \hat{\kappa}_m^2 \right)$$

$$= S(f)^2 \frac{\|\kappa\|^2}{h^{2q+1}} \sum_{k,k'=1}^K \mu_k \mu_{k'} \left(\sum_{n=1}^N |\nu_n^{(k)}|^2 |\nu_n^{(k')}|^2 \right). \quad (12)$$

The first line is valid to $\mathcal{O}(1/(mh)^4) + \mathcal{O}(Km/N)$, so we Taylor expand $\nu_{n+m}^{(k)}$ for $|mh| < \mathcal{O}((Nh/K)^{1/5})$ and drop all terms with $|mh| > \mathcal{O}((Nh/K)^{1/4})$. The resulting expression is accurate to $\mathcal{O}_{\mathcal{R}}((K/Nh)^{4/5})$. The final line follows from Parseval's identity. \square

For $K = 1$, Eq. (12) reduces to the well known result [15] for the variance of smoothed tapered periodogram:

$$\mathbf{Var} \left[\frac{1}{h^{q+1}} \int \kappa \left(\frac{f-f'}{h} \right) |\zeta_{\nu}(f')|^2 df' \right] \simeq \frac{S(f)^2 \|\kappa\|^2}{h^{2q+1}} \sum_{n=1}^N \nu_n^4, \quad (13)$$

where $\zeta_{\nu}(f)$ is the tapered Fourier transform. In (13), $\sum_{n=1}^N \nu_n^4$ is $\mathcal{O}(1/N)$. For the sinusoidal tapers, (12) can be explicitly evaluated:

$$\mathbf{Var} \left[\widehat{\partial_f^q S}_{\kappa}(f) \right] \simeq \frac{\|\kappa\|^2 S(f)^2}{Nh^{q+1}} \left(1 + \frac{1}{2K} \right) + \mathcal{O}_{\mathcal{R}} \left(\left(\frac{h}{K} \right)^2 \right) + \mathcal{O}_{\mathcal{R}} \left(\left(\frac{K}{Nh} \right)^{4/5} \right), \quad (14)$$

where we have used

$$\frac{1}{K^2} \sum_{k,k'=1}^K \sum_{n=1}^N |\nu_n^{(k)}|^2 |\nu_n^{(k')}|^2 = \frac{4}{K^2(N+1)^2} \sum_{k,k'=1}^K \sum_{n=1}^N \sin^2 \left(\frac{\pi kn}{N+1} \right)^2 \sin^2 \left(\frac{\pi k'n}{N+1} \right)^2 = \frac{2K+1}{2K(N+1)}. \quad (15)$$

4 SMOOTHED LOG MULTI-TAPER ESTIMATE

We now show that combining kernel smoothing with *multi-tapering* does improve the estimation of the logarithm of the spectral density, $\theta(f) = \ln[S(f)]$. Let

$$\widehat{\partial_f^q \theta}_{\kappa}(f) \equiv \frac{1}{h^{q+1}} \int_{-\frac{1}{2}}^{\frac{1}{2}} \kappa \left(\frac{f-f'}{h} \right) \hat{\theta}_{mt}(f') df'. \quad (16)$$

For $h \ll 1$, and $Nh \gg 1$, we expand (16) in the bandwidth

$$\mathbf{Bias}[\widehat{\partial_f^q \theta}_{\kappa}(f)] \simeq B_p \partial_f^p \theta(f) h^{p-q} + \partial_f^q [|\theta''(f)| + |\theta'(f)|^2] \frac{K^2}{24N^2}. \quad (17)$$

The first term is the bias from kernel smoothing and the second term is from the sinusoidal multi-taper estimate (8). Traditionally, the ‘‘delta approximation’’, $\mathbf{Var}[f(X)] = f'(\mathbf{E}[X])^2 \mathbf{Var}[X]$, is used to evaluate the variance of the smoothed log-periodogram. For the delta approximation to be valid, the characteristic scale of variation of $f(\cdot)$ must be large relative to $\sqrt{\mathbf{Var}[X]}$, where f is continuously differentiable. This requirement is not fulfilled for the log-periodogram, and the resulting analysis makes an order one error in single taper estimation. For the multi-taper estimation, the expansion parameter

for the delta approximation is $1/K$. To leading order in the $1/K$ expansion, the variance inflation factor from the long tail of the $\ln[\chi_{2K}^2]$ distribution is not visible. Recall that $\mathbf{Var}[\hat{\theta}_{mt}(f')] \approx [K\psi'(K)] \times \mathbf{Var}[\hat{S}_{mt}(f')]/S(f)^2$ for $|f - f'| \ll 1$. We believe that adding a $K\psi'(K)$ correction improves the accuracy of the delta approximation for $f'' \neq f'$. Therefore, we evaluate the variance of the smoothed log multi-taper estimate by using the approximate identity:

$$\mathbf{Cov}[\hat{\theta}_{mt}(f'), \hat{\theta}_{mt}(f'')] \approx \frac{[K\psi'(K)]}{S(f)^2} \times \mathbf{Cov}[\hat{S}_{mt}(f'), \hat{S}_{mt}(f'')] , \quad (18)$$

for $|f' - f| \ll 1$ and $|f'' - f| \ll 1$. Using (18), the variance of $\hat{\theta}(f)$ is

$$\mathbf{Var}[\widehat{\partial_f^q \theta}_\kappa(f)] \simeq \frac{K\psi'(K)}{S(f)^2 h^{2(q+1)}} \int_{-\frac{1}{2}}^{\frac{1}{2}} \int_{-\frac{1}{2}}^{\frac{1}{2}} \kappa\left(\frac{f-f'}{h}\right) \kappa\left(\frac{f-f''}{h}\right) \mathbf{Cov}[\hat{S}_{mt}(f'), \hat{S}_{mt}(f'')] df' df'' . \quad (19)$$

Thus, the variance of $\widehat{\partial_f^q \theta}(f)$ reduces to the same calculation as the variance of $\widehat{\partial_f^q S}(f)$:

$$\mathbf{Var}[\widehat{\partial_f^q \theta}_\kappa(f)] \simeq \frac{(K + \frac{1}{2})\psi'(K)\|\kappa^2\|}{Nh^{2q+1}} + \mathcal{O}_{\mathcal{R}}\left(\frac{1}{K}\right) + \mathcal{O}_{\mathcal{R}}\left(\left(\frac{K}{Nh}\right)^{4/5}\right) , \quad (20)$$

for the uniformly weighted sinusoidal tapers. (See the calculation in Theorem 3.1.) Combining (17) with (19) yields the expected asymptotic square error (EASE) in $\widehat{\partial_f^q \theta}_\kappa$:

Theorem 4.1 *Let $S(f)$ have p continuous derivatives. Consider the two-stage estimate (16) using the uniformly weighted sinusoidal tapers in the first-stage. Under the hypotheses of Theorem 3.1 and the formal approximation (18), the expected asymptotic square error of $\widehat{\partial_f^q \theta}_\kappa$ is*

$$\mathbf{E}\left[|\widehat{\partial_f^q \theta}_\kappa(f) - \partial_f^q \theta(f)|^2\right] \approx \left[B_p \partial_f^p \theta(f) h^{p-q} + \partial_f^q [\theta''(f) + |\theta'(f)|^2] \frac{K^2}{24N^2} \right]^2 + \frac{(K + \frac{1}{2})\psi'(K)\|\kappa\|^2}{Nh^{2q+1}} + \mathcal{O}_{\mathcal{R}}\left(h^{2(p-q)+1}\right) + \mathcal{O}_{\mathcal{R}}\left(\frac{1}{K}\right) + \mathcal{O}_{\mathcal{R}}\left(\left(\frac{K}{Nh}\right)^{4/5}\right) . \quad (21)$$

The benefit of multi-tapering (in terms of the variance reduction) is significant for using a 2 to 20 tapers. However, the marginal benefit of each additional taper tends rapidly to zero. Minimizing (21) with respect to h and K yields the following result:

Corollary 4.2 *Under the hypotheses of Theorem 4.1, the expected asymptotic square error (EASE) of $\widehat{\partial_f^q \theta}_\kappa$ is minimized by*

$$h_o(f) = \left[\frac{2q+1}{2(p-q)} \frac{(K + \frac{1}{2})\psi'(K)\|\kappa\|^2}{B_p^2 N |\partial_f^p \theta(f)|^2} \right]^{\frac{1}{2p+1}} , \quad (22)$$

and

$$B_p [\partial_f^p \theta(f)] \{ \partial_f^q [\theta''(f) + |\theta'(f)|^2] \} K_{opt}^3 \simeq 6 \|\kappa\|^2 N h_o^{-(p+q+1)} . \quad (23)$$

Thus $h_{opt} \sim N^{-1/(2p+1)}$ and $K_{opt} \sim N^{(3p+q+2)/(6p+3)}$. For kernels of order $(0, 2)$, this reduces to $h_{opt} \sim N^{-1/5}$ and $K_{opt} \sim N^{8/15}$. Thus the ordering $1 \ll K \ll Nh$ is justified. The EASE (21) 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 (22), the leading order EASE reduces to

$$\mathbf{E} \left[\left| \widehat{\partial_f^q \theta}(f_j) - \partial_f^q \theta(f_j) \right|^2 \right] \simeq M_{q,p} |B_p \partial_f^p \theta(f_j)|^{\frac{2(2q+1)}{(2p+1)}} \left(\frac{(K + \frac{1}{2}) \psi'(K) \|\kappa\|^2}{N} \right)^{\frac{2(p-q)}{(2p+1)}}, \quad (24)$$

where $M_{q,p} \equiv \left(\frac{2q+1}{2(p-q)}\right)^{\frac{2(p-q)}{(2p+1)}} + \left(\frac{2(p-q)}{2q+1}\right)^{\frac{(2q+1)}{(2p+1)}}$. Thus the EASE in estimating $\partial_f^q \theta$ is proportional to $N^{-\frac{2(p-q)}{(2p+1)}}$. We note that if $K = 1$ (a single taper), the variance term in (21) is inflated by a factor of $\frac{\pi^2}{6} \sum_{n=1}^N \nu_n^4$. Thus using a moderate level of multi-tapering prior to smoothing the logarithm reduces the EASE by a factor of $[\frac{\pi^2}{6} \sum_{n=1}^N \nu_n^4]^{4/5} = [\frac{\pi^2}{4}]^{4/5}$, where we substitute $\sum_{n=1}^N \nu_n^4 = 1.5$ for the sinusoidal tapers.

From (24), using the best fixed halfwidth kernel smoother degrades performance by a factor of

$$\frac{\text{EASE}(h_{global})}{\text{EASE}(h_{variable})} = \left[\int_{-\frac{1}{2}}^{\frac{1}{2}} |\theta''(f)|^2 df \right]^{1/5} \bigg/ \int_{-\frac{1}{2}}^{\frac{1}{2}} |\theta''(f)|^{2/5} df \quad (25)$$

over using an optimal variable halfwidth smoother [4]. In many cases, the spectral range is large, and thus it is often essential to allow the bandwidth to vary locally as a function of frequency.

Equation (22) gives an explicit solution for the bandwidth which minimizes the local bias versus variance trade-off. It shows that when $\theta(f)$ is rapidly varying ($|\theta''(f)|$ is large), then the kernel bandwidth should be decreased. However, (22) has two major difficulties. First, (21)-(24) are based on a Taylor series expansion and the expansion parameter is $h_o \sim 1/N^{1/(2p+1)}$. Even when $1/N$ is small, $(1/N)^{1/(2p+1)}$ may be not so small. Second, $\theta''(f)$ and $h_o(f)$ are unknown and need to be estimated.

5 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 made prior to estimating $\theta(f)$. To simplify the implementation, we choose K independent of frequency, and usually set $K \approx cN^{8/15}$, where c is a constant. For nonparametric function estimation, data adaptive multiple stage schemes are given in [1, 4, 11]. A straightforward application of these schemes to multi-taper spectral estimation has the following steps:

0) Evaluate the multi-taper estimate of (3) on a grid of size $2N+2$. If the computational effort is not important, set $K = N^{8/15}$; otherwise choose K according to your computational budget.

1a) Kernel smooth $\hat{\theta}_{mt}(f)$ with a kernel of order (0,4) for a number of different bandwidths, h_ℓ , and evaluate the average square residual (ASR) as a function of h_ℓ :

$$ASR(h_\ell) = \sum_{n=1}^N |\hat{\theta}_{st}(f_n) - \hat{\theta}_\kappa(f_n|h_\ell)|^2, \quad (26)$$

where $\hat{\theta}_\kappa(f_n|h_\ell)$ is the kernel estimate of $\theta(f)$ using bandwidth h_ℓ applied to $\hat{\theta}_{mt}(f)$, while $\hat{\theta}_{st}(f_n)$ is the single taper estimate: $\hat{\theta}_{st}(f) = \ln[|\zeta(f + \Delta) - \zeta(f - \Delta)|^2/2(N + 1)] + .577$.

1b) Estimate the optimal (0,4) global halfwidth using a goodness of fit method. Relate this to the optimal (2,4) using the halfwidth quotient relation. (See below.)

2) Estimate $\theta''(f)$ by smoothing the multi-taper estimate with global halfwidth $h_{2,4}$.

3) Estimate $\theta(f)$ by substituting $\hat{\theta}''(f)$ into the optimal halfwidth expression corresponding to the minimum of (14).

For Step 1b), Müller and Stadtmüller propose to determine the starting halfwidth by minimizing the Rice criterion. In [11], we describe a different method for selecting the initial bandwidth in step 1b). Our method is based on fitting the average square residual of (26) to a parametric expression based on (21). This parametric fit usually outperforms the Rice criterion because it uses an asymptotically valid expression.

In (26), the ASR is computed relative to the single taper estimate, $\hat{\theta}_{st}(f_n)$, instead of the multi-taper estimate, $\hat{\theta}_{mt}(f_n)$. We do this because the multi-taper estimate is strongly autocorrelated for frequencies, f and f' with $|f - f'| \leq K/2N$. To correct for using $\hat{\theta}_{st}(f)$ in step 1 and $\hat{\theta}_{mt}(f)$ in steps 2 and 3, we inflate the variance in the (0,4) kernel estimate. The halfwidth quotient relation relates the optimal halfwidth for derivative estimates, $\hat{h}_{2,4}$ to the optimal halfwidth for a (0,4) kernel using (22):

$$\hat{h}_{2,4} = H(\kappa_{2,4}, \kappa_{0,4})\hat{h}_{0,4}, \quad \text{where } H(\kappa_{2,4}, \kappa_{0,4}) \equiv \left(\frac{10B_{0,4}^2 \|\kappa_{2,4}\|^2}{B_{2,4}^2 \|\kappa_{0,4}\|^2} \right)^{\frac{1}{9}} \left(\frac{\pi^2 N \sum_n |\nu_n^{(1)}|^4}{6} \right)^{\frac{1}{9}}. \quad (27)$$

The last term in parentheses is the variance inflation factor from using a single taper. To minimize the effects of tapering-induced autocorrelation, we recommend using a Tukey taper for $\hat{\theta}_{st}$.

When $\hat{\theta}''(f)$ is vanishingly small, the optimal halfwidth becomes large. Thus, $\hat{h}_{0,2}$ needs to be regularized. Following [11], we determine the size of the regularization from $\hat{h}_{0,4}$ in the previous stage.

We say a “plug-in” scheme has a relative convergence rate of $N^{-\alpha}$ if

$$\mathbf{E} \left[|\hat{\theta}(f|\hat{h}_{0,2}) - \theta(f)|^2 \right] \simeq \left(1 + \mathcal{O}(C_r^2 N^{-2\alpha}) \right) \mathbf{E} \left[|\hat{\theta}(f|h_{0,2}) - \theta(f)|^2 \right],$$

where $h_{0,2}$ is the optimal halfwidth and $\hat{h}_{0,2}$ is the estimated halfwidth. In [1], a detailed analysis of the convergence properties of their similar scheme is given. Their scheme has an optimal convergence rate of $N^{-4/5}$ and a relative convergence rate of $N^{-1/4}$. Our simpler

method has the same convergence rate of $N^{-4/5}$ and a slightly slower relative convergence rate: $N^{-2/9}$.

6 COMPARISON OF KERNEL SMOOTHER ESTIMATES

We now compare three different kernel smoother estimates of the log-spectrum: 1) Kernel smoothing the log-multitaper estimate, $\hat{\theta}_{mt}$ as in (16); 2) Kernel smoothing the log-single taper estimate, $\ln[\hat{S}_{st}]$; 3) The logarithm of the kernel smoothed multi-taper spectral estimate, $\ln[\hat{S}_\kappa]$ as in (21). In all cases, we use a variable halfwidth kernel smoother with the initial $h_{0,4}$ halfwidth estimated by the fitted square residual method as described in Sec. 5 and the appendix.

We use the moving average time series model which was considered in [6]: $x_t = e_t - 0.3e_{t-1} - 0.6e_{t-2} + 0.3e_{t-3}$, where e_t is a zero mean, unit variance, uncorrelated Gaussian process. We compute the integrated square error (ISE): $\int |\hat{\theta}(f) - \theta(f)|^2 df$, averaged over 500 realizations for time series lengths of 128 and 1024. We use the sinusoidal tapers and choose $K = (N/2)^{8/15}$, which is $K = 9$ for $N = 128$ and $K = 28$ for $N = 1024$. Table 1 summarizes our simulation:

Error Criterion	MISE	MaxISE	MISE	MaxISE
Method	$N = 128$	$N = 128$	$N = 1024$	$N = 1024$
Smoothed log-multi-taper (16)	.453	.694	.186	.515
Log of smoothed multi-taper (9)	.483	.743	.195	.515
Smoothed log-single taper	.622	1.009	.209	.842

Table 1: Integrated square error averaged over 500 realizations where MaxISE is the integrated square error for the worst of the 500 realizations.

The simulation shows that smoothing before taking the logarithm of the multitaper estimate performs somewhat more poorly than smoothing the log multi-tapered estimate. The performance degradation is 6.6 % for $N = 128$ and 4.8 % for $N = 1024$. The performance differential is due to the presence of broad-band bias error. As N increases, the smoothing halfwidth decreases and the effects of broad-band bias will shrink. For more peaked spectral densities, N may have to be quite large before the two estimates perform similarly.

In comparing the first and third estimates, we expect to see an improvement factor of $[\frac{\pi^2}{4}]^8$ for multi-tapering. Multi-tapering prior to smoothing the logarithm reduces the ISE by more than expected. We attribute this additional reduction to the poor performance of automatic halfwidth selection criteria in the presence of strong noise. Note that using a single taper is very nonrobust in the sense that the worst realizations have much larger ISEs than do either of the other two methods. Our simulations also indicate that the optimal number of tapers grows at faster than $N^{8/15}$ for our particular spectrum and $100 < N < 1000$.

7 REMARKS

1) P. Bloomfeld (private correspondence) points out that a similar variance reduction can be achieved by pre-smoothing the periodogram before transforming to the logarithmic scale and smoothing again. Our analysis in Sec. III shows the optimal amount of pre-smoothing. Note multi-tapering offers broad-band bias protection with asymptotically no variance inflation. In contrast, pre-smoothing the tapered periodogram inflates the variance by $\sum_n |\nu_n|^4$. For the pre-smoothing algorithm to be as efficient as multi-tapering, the amount of tapering needs to go to zero as $N \rightarrow \infty$.

2) Pawitan and O’Sullivan [6] advocate a penalized Whittle likelihood estimate with generalized cross-validation. Clearly, it should be advantageous to use an approximation of the likelihood. Unfortunately, the penalized likelihood approach corresponds to a *fixed* halfwidth kernel and does not reduce the strength of the smoothing near the points of rapid spectral variation. We expect a variable halfwidth kernel smoother to outperform a penalized likelihood method by the factor given in (25). Also note that the Whittle likelihood is asymptotic and provides with no information on the amount of tapering which should be done in a finite sample size.

3) An early adaptive multi-taper scheme was proposed in [13]. This scheme makes the unrealistic assumption that the spectral density is $S(f)$ in the region $[f - W, f + W]$ and is $(\sigma^2 - 2WS(f))/(1 - 2W)$ elsewhere, where W is a bandwidth parameter and σ^2 is the variance. Furthermore, the adaptive weighting of [13] is usually computed with the Slepian tapers, which have a fixed bandwidth, W . The goal of adaptive methods, to reduce the bandwidth of the estimate when the spectrum is rapidly varying, is defeated by the inflexibility of the Slepian tapers. In our previous simulations [10, 12], the adaptive weighting of [13] has performed so poorly that we no longer consider it a viable alternative.

4) The evolutionary spectrum of Priestley [8] can be estimated by applying a two dimensional kernel smoother (in the time-frequency plane) to the log-multi-tapered spectrogram (Riedel [9]).

8 SUMMARY

We have analyzed the expected asymptotic square error of the smoothed log multi-tapered periodogram and shown that multi-tapering reduces the error by a factor of $[\frac{\pi^2}{4}]^{\frac{4}{5}}$ for the sinusoidal tapers. The optimal rate of pre-smoothing prior to taking logarithms is $K \sim N^{8/15}$, but the expected loss depends only weakly on K when $1 \ll K \ll Nh$. A similar enhancement in performance has been reported by Walden [16] for estimating the innovations variance: $\exp [f \ln[S(f)]df]$.

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 by using the

iteration method of [2]. Our multiple stage estimate has the following steps: 1) Estimate the optimal kernel halfwidth for a kernel of (0,4) for the log-single tapered periodogram. 2) Estimate $\hat{\theta}_{mt}(f) \equiv \ln[\hat{S}_{mt}(f)] - B_K$ as described in Sec. 2. 3) Estimate $\theta''(f)$ using a kernel smoother of order (2,4). 4) Estimate $\theta(f)$ using a kernel smoother of order (0,2) with the halfwidth $h_0(f) \approx c|\widehat{\partial_f^2 \theta}|^{-2/5} N^{-1/5}$.

APPENDIX: FITTED SQUARE RESIDUAL INITIALIZATION

The factor method (27) relates the optimal halfwidth for a (2,4) kernel to that of a (0,4) kernel. To begin the kernel estimation, a halfwidth for the (0,4) kernel needs to be specified. In [4], Müller and Stadtmüller propose to select $h_{0,4}$ using a penalized goodness of fit (GoF) method such as generalized cross-validation or the Rice criterion. In penalized goodness of fit methods, the (0,4) halfwidth is chosen by minimizing a functional of Nh and $ASR(h)$ (26).

Unfortunately, these GoF functionals are often flat near their minimum and the actual minimum can be very sensitive to noise. As a result, the halfwidth given by the GoF methods tends to vary appreciably even when the noise is weak. Furthermore, when tapering or multitapering is used, the residual errors are correlated and GoF methods have great difficulty estimating the optimal halfwidth. To remedy this sensitivity problem, we fit $ASR(h)$ to a two parameter model prior to estimating the optimal bandwidth [11].

The fitted residual error method [11] begins by evaluating the average square residual (ASR) (26) as a function of the kernel halfwidth. (GoF methods also evaluate $ASR(h)$.) For the (0,4) kernel, the bias error is proportional to h^4 our parametric model is

$$ASR(h) \sim aV(h) + bh^8, \tag{A1}$$

where $V(h) = \sum_{j=1}^N (\mu_j(h) - \delta_{0,j})^2$ with $\mu_j(h) = \kappa(j/Nh)/h$. In the large Nh limit, $V(h) \approx 1 + [||\kappa||^2 - 2\kappa(0)]/Nh$. Equation (A1) represents the integral of (21) over frequency. The first term corresponds to the bias, $\int |B_p \partial_f^p \theta|^2 df$, and the second term corresponds to the variance. The model has two parameters, a and b . (Note that for smoothing the log-tapered periodogram of a Gaussian time series, $a = 1$.)

By parameterizing $ASR(h)$ with (A1), we are assured of an unique minimum. The variance of $ASR(h)$ is of order $\frac{1}{N}$ and is practically independent of h . We determine a, b by minimizing the weighted least squares problem:

$$\{a, b\} = \operatorname{argmin}_{\{a, b\}} \sum_{h_j} \left[ASR(h_j) - \left(aV(h_j) + bh_j^8 \right) \right]^2, \tag{A2}$$

where we use an equi-spaced grid in h . The upper and lower limiting bandwidths, h_U and h_L , for the grid in h is chosen such that $ASR(h_U) \approx 2ASR(h_{min}) \approx ASR(h_L)$. The least squares fit in (A2) is heuristic because the residual error are correlated for different values of h .

The *ASR* measures the difference between the measured values and the prediction based on the same measured values. We wish to minimize the difference between the predicted values and new measurements. The expected value of the *ASR* differs from the EASE (21) by a function of Nh . We then choose the halfwidth which minimizes our parameterized model of the EASE: $h_{opt} = (a\|\kappa\|^2/8b)^{1/9}$. We caution that the theoretical convergence properties of this estimator are unknown. Nevertheless, our simulations show that this fitting procedure gives more stable halfwidth estimates than penalized goodness of fit methods do. The advantage of the fitted residual error method appears even larger when the residuals are correlated from tapering.

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