

# A unified view of multitaper multivariate spectral estimation

BY A. T. WALDEN

*Department of Mathematics, Imperial College of Science, Technology and Medicine,  
180 Queen's Gate, London SW7 2BZ, U.K.*

a.walden@ic.ac.uk

## SUMMARY

The orthogonal multitaper framework for cross-spectral estimators provides a simple unifying structure for determining the corresponding statistical properties. Here cross-spectral estimators are represented by a weighted average of orthogonally-tapered cross-periodograms, with the weights corresponding to a set of rescaled eigenvalues. Such a structure not only encompasses the Thomson estimators, using Slepian and sine tapers, but also Welch's weighted overlapped segment averaging estimator and lag window estimators including frequency-averaged cross-periodograms. The means, smoothing and leakage biases, variances and asymptotic distributions of such estimators can all be formulated in a common way; comparisons are made for a fixed number of degrees of freedom. The common structure of the estimators also provides a necessary condition for the invertibility of an estimated cross-spectral matrix, namely that the weight matrix of the estimator written in bilinear form must have rank greater than or equal to the dimension of the cross-spectral matrix. An example is given showing the importance of small leakage and thus illustrating that the various estimators need not be equivalent in practice.

*Some key words:* Cross-spectrum; Lag-window; Multiple coherence; Multitapering; Segment averaging; Wishart distribution.

## 1. INTRODUCTION

Estimation of the elements of the cross-spectral matrix for a set of stationary time series is a widely used statistical procedure throughout the sciences, providing not only spectral but, after matrix inversion, important frequency domain quantities such as partial and multiple coherence. Thomson (1982) introduced a form of spectral and cross-spectral estimation built around averages of multiply-tapered periodograms or cross-periodograms. These estimators are intuitively very appealing (Percival & Walden, 1993), but have sometimes been considered to be nothing but a reformulation of Welch's weighted overlapped segment averaging estimator or indeed roughly equivalent to traditional lag window estimators (McCloud, Scharf & Mullis, 1999).

This paper demonstrates that the orthogonal multitaper framework for cross-spectral estimators provides a simple unifying structure for examining the statistical properties of commonly encountered estimators. Section 2 develops the representation of cross-spectral estimators in terms of a weighted average of orthogonally-tapered cross-periodograms, with the weights corresponding to a set of rescaled eigenvalues. The means, smoothing and leakage biases, variances and asymptotic distributions of such estimators are formulated in a common way in § 3.

As shown in § 4, such a representation not only encompasses the Thomson estimators, using Slepian and sine tapers, but also Welch's weighted overlapped segment averaging estimator and lag window estimators including frequency-averaged cross-periodograms. Smoothing and leakage bias and spectral window comparisons are made within this framework by fixing the number of degrees of freedom of the estimator. In § 5 it is shown that the common structure of the estimators also provides a necessary condition for the invertibility of estimated cross-spectral matrices for uses such as coherence estimation. Finally in § 6 an example is given showing the importance of small leakage, thus illustrating that differences between the estimators can be critical and hence that the various estimators are not all equivalent in practice.

## 2. ORTHOGONAL MULTITAPER CROSS-SPECTRUM ESTIMATORS

### 2.1. Background

Let  $\{X_l(t)\}$  ( $l = 1, \dots, L$ ) denote a set of  $L$  real-valued zero-mean second-order stationary processes which are also jointly stationary; that is  $s_{lm}(\tau)$ , the covariance between  $X_l(t + \tau)$  and  $X_m(t)$ , depends only on  $\tau$ . Provided  $\sum_{\tau} |s_{lm}(\tau)| < \infty$  ( $l, m = 1, \dots, L$ ) as assumed throughout, then the cross-spectrum between any two series  $\{X_l(t)\}$  and  $\{X_m(t)\}$  exists and is defined as

$$S_{lm}(f) = \Delta \sum_{\tau=-\infty}^{\infty} s_{lm}(\tau) e^{-i2\pi f\tau\Delta}, \quad |f| \leq f_N,$$

where  $\Delta$  is the sample interval and  $f_N = 1/(2\Delta)$  is the Nyquist frequency. This is the  $(l, m)$ th element of the cross-spectral matrix  $S(f)$ . For a fixed frequency  $f$  such that  $0 \leq f \leq f_N$ , let us define the complex demodulate of the original process by  $Z_l(t) \equiv X_l(t) \exp(i2\pi ft\Delta)$ , which corresponds to shifting all the frequency components of  $\{X_l(t)\}$  by  $f$ . The process  $\{Z_l(t)\}$  is also a zero-mean stationary process. We consider cross-spectrum estimators which are bilinear forms of any two series  $\{X_l(t)\}$ ,  $\{X_m(t)\}$  (Bloomfield, 1976, p. 241). In particular we consider the class of bilinear estimators which can be written

$$\hat{S}_{lm}(f) = \Delta \sum_{s=1}^N \sum_{t=1}^N X_l(s) Q(s, t) e^{i2\pi f(t-s)\Delta} X_m(t) = \Delta Z_l^H Q Z_m, \quad (1)$$

where superscript  $H$  denotes complex-conjugate transpose,  $Z_l$  is the column vector of  $Z_l(1), \dots, Z_l(N)$  values, and the elements  $Q(s, t)$  of the weight matrix are real-valued, are not functions of frequency and do not depend on  $\{Z_l(t)\}$  or  $\{Z_m(t)\}$ . Additionally, the estimator must satisfy the same property as the true cross-spectrum, namely  $\hat{S}_{lm}(f) = \hat{S}_{ml}^H(f)$ . However,  $\hat{S}_{ml}^H(f) = \Delta Z_l^H Q^H Z_m$  and a comparison with (1) shows that  $Q = Q^H$  and, since  $Q$  is real,  $Q$  must be symmetric.

In order that the estimator is nonnegative real when  $l = m$ ,  $Q$  must also be positive semidefinite, that is  $\hat{S}_{ll}(f) = \Delta Z_l^H Q Z_l \geq 0$  ( $l = 1, \dots, N$ ); in this case Grenander & Rosenblatt (1984, p. 129) show that for any linear process there exists an estimator with a Toeplitz form for  $Q$  having mean squared error that is asymptotically not larger than that of an asymptotically unbiased estimator with non-Toeplitz form for  $Q$ .

The spectral decomposition of a real symmetric positive semidefinite matrix gives

$$Q = \sum_{k=0}^{N-1} \lambda_k u_k u_k^H,$$

where the real-valued column vectors  $u_k$  ( $k = 0, \dots, N - 1$ ) are the eigenvectors of  $Q$ , and

$\lambda_k \geq 0$  ( $k = 0, \dots, N - 1$ ) are the corresponding real eigenvalues. Here  $u_k$  is the column vector of  $u_k(1), \dots, u_k(N)$  values. From (1),

$$\hat{S}_{lm}(f) = \Delta \sum_{k=0}^{N-1} \lambda_k \left\{ \sum_{s=1}^N u_k(s) X_l(s) e^{-i2\pi f s \Delta} \right\} \left\{ \sum_{t=1}^N u_k(t) X_m(t) e^{i2\pi f t \Delta} \right\}. \tag{2}$$

The system is normalised so that  $\|u_k\|^2 = 1$  ( $k = 0, \dots, N - 1$ ). We note that each component of the sum is weighted by the  $k$ th eigenvalue of  $Q$ . Since we are assuming  $Q$  to be positive semidefinite, its rank  $K$  can be taken to satisfy  $1 \leq K \leq N$ ; we assume  $K > 0$ . Then, for  $K < N$ ,  $\lambda_K = \dots = \lambda_{N-1} = 0$ , and, if we define  $\lambda_k \equiv \gamma_k/K$ ,  $h_k(t) \equiv u_k(t)\gamma_k^{1/2}$  ( $k = 0, \dots, K - 1$ ), then the cross-spectrum estimator can be written more simply as

$$\hat{S}_{lm}(f) = \frac{\Delta}{K} \sum_{k=0}^{K-1} \gamma_k \left\{ \sum_{s=1}^N u_k(s) X_l(s) e^{-i2\pi f s \Delta} \right\} \left\{ \sum_{t=1}^N u_k(t) X_m(t) e^{i2\pi f t \Delta} \right\} \tag{3}$$

$$= \frac{\Delta}{K} \sum_{k=0}^{K-1} \left\{ \sum_{s=1}^N h_k(s) X_l(s) e^{-i2\pi f s \Delta} \right\} \left\{ \sum_{t=1}^N h_k(t) X_m(t) e^{i2\pi f t \Delta} \right\}. \tag{4}$$

Hence all bilinear estimators of the form (1) with a real-valued, symmetric, positive semidefinite matrix  $Q$  of weights can be written as an average of  $K$  direct cross-spectrum estimators;  $K$  is the rank of  $Q$ . The data taper of the  $k$ th estimator is defined by  $\{h_k(t) \equiv u_k(t)\gamma_k^{1/2}\}$ .

### 2.2. Multitaper multivariate spectrum estimator

Let  $X(t)$  denote the real-valued column vector with components  $X_1(t), \dots, X_L(t)$ . For  $k = 0, \dots, K - 1$  we define the column vector  $J_k(f)$  to be the vector Fourier transform with the same eigenvector values  $u_k(t)$  multiplying all components of  $X(t)$ . Then

$$J_k(f) \equiv \Delta^{\frac{1}{2}} \sum_{t=1}^N u_k(t) X(t) e^{-i2\pi f t \Delta}.$$

By the spectral representation theorem (Brockwell & Davis, 1991, p. 405) the real-valued column vector  $X(t)$  can be written

$$X(t) = \int_{-f_N}^{f_N} e^{i2\pi f' t \Delta} dZ(f'),$$

where the components  $dZ_1(f), \dots, dZ_L(f)$  of  $dZ(f)$  are individually orthogonal and jointly cross-orthogonal:

$$E\{dZ_l(f') dZ_m^H(f)\} = \begin{cases} S_{lm}(f) df & \text{if } f = f', \\ 0 & \text{otherwise.} \end{cases}$$

Each  $X_l(t)$  ( $l = 1, \dots, L$ ) is real, so that  $X_l(t) = X_l^H(t)$  and thus  $dZ_l(f) = dZ_l^H(-f)$ . Now

$$J_k(f) = \Delta^{-\frac{1}{2}} \int_{-f_N}^{f_N} U_k(f - f') dZ(f'), \tag{5}$$

where

$$U_k(f) \equiv \Delta \sum_{t=1}^N u_k(t) e^{-i2\pi f t \Delta}.$$

From (3) the estimator of the  $L \times L$  cross-spectral matrix  $S(f)$  is given by

$$\hat{S}(f) = \frac{1}{K} \sum_{k=0}^{K-1} \gamma_k J_k(f) J_k^H(f). \quad (6)$$

Equation (6) defines a multitaper multivariate spectral estimator. For  $j, k = 0, \dots, K-1$ , the orthogonality properties of the  $dZ(f)$  components give

$$\text{cov}\{J_j(f), J_k(f)\} = E\{J_j(f) J_k^H(f)\} = \frac{1}{\Delta} \int_{-f_N}^{f_N} U_j(f-f') U_k^H(f-f') S(f') df'. \quad (7)$$

Setting  $j = k$  we have

$$E\{J_k(f) J_k^H(f)\} = \frac{1}{\Delta} \int_{-f_N}^{f_N} |U_k(f-f')|^2 S(f') df',$$

and hence, from (6),

$$E\{\hat{S}(f)\} = \int_{-f_N}^{f_N} U(f-f') S(f') df',$$

with

$$U(f) \equiv \frac{1}{K\Delta} \sum_{k=0}^{K-1} \gamma_k |U_k(f)|^2. \quad (8)$$

The function  $U(f)$  is the overall spectral window of the multitaper estimator.

The eigenvectors  $u_k$  and nonnegative eigenvalues  $\gamma_k$  are the key ingredients which differentiate between different cross-spectrum estimators. Their joint form governs the overall spectral window  $U(f)$  and the smoothing and leakage biases discussed in § 3.1, while the disposition of the  $\gamma_k$  alone determine the equivalent degrees of freedom of the estimator. Moreover, as shown in § 5, the number of nonzero eigenvalues must be greater than or equal to the number of processes,  $L$ , if the estimated cross-spectrum matrix is to be invertible.

### 2.3. Properties of the tapers and their Fourier transforms

Here we list properties of the tapers  $u_k$  and their Fourier transforms  $U_k(\cdot)$  of which use will be made throughout the paper. The first three properties follow automatically from the definitions. Property (iv) follows from a suitable scaling of  $Q$  and is justified in § 3.1. Property (v) is sufficient to guarantee asymptotic unbiasedness and in § 4 is justified for all the cross-spectrum estimators of interest to us. Condition (vi) is required only for the asymptotic distribution results of § 3.3 and in § 4 is proved for some of the cross-spectrum estimators of interest to us. Finally, property (vii) is a practical, rather than theoretical, design requirement involving the choice of the resolution bandwidth. The following items will be referred to in the paper as 'taper property (i)' and so on.

(i) We require that  $\{u_k, k = 0, \dots, K-1\}$  are orthonormal.

(ii) We require that  $\{U_k(\cdot), k = 0, \dots, K-1\}$  are periodic with period  $1/\Delta$ .

(iii) Since  $Q$  is symmetric, the real tapers, when centred, are either symmetric or skew-symmetric. The corresponding Fourier transforms are thus symmetric or skew-symmetric respectively. When ordered by corresponding distinct eigenvalues, the eigenvectors are automatically alternately symmetric or skew-symmetric; if the eigenvalues are not distinct, the eigenvectors are forcibly ordered to be alternately symmetric or skew-symmetric.

(iv) The overall spectral window  $U(f)$  is periodic with period  $1/\Delta$  and integrates to unity over  $-f_N$  to  $f_N$ .

(v) For  $k = 0, \dots, K - 1$ , each  $|U_k(f)|^2$  behaves like  $\Delta\delta(f)$ , where  $\delta(\cdot)$  is the Dirac delta, as  $N \rightarrow \infty$ . Hence, for each taper the designed resolution bandwidth  $2W$ , say, decreases with increasing sample size; that is  $W \rightarrow 0$  as  $N \rightarrow \infty$ .

(vi) The discrete tapers  $\{u_k, k = 0, \dots, K - 1\}$  correspond to sampling  $K$  rescaled bounded taper functions, each with support on the same finite-length interval of the real line, with the taper functions enjoying orthonormality properties on this finite interval.

(vii) The designed resolution band, namely  $|f| \leq W$ , within which each individual  $|U_k(\cdot)|$  and the overall spectral window  $U(\cdot)$  are concentrated, is assumed to have been chosen narrow enough to ensure the components of  $S(f)$  are essentially constant across it; Jenkins & Watts (1968, p. 280) call this empirical design procedure ‘window closing’ and the issue is explored in detail in Percival & Walden (1993).

### 3. STATISTICAL PROPERTIES

#### 3.1. Biases

If  $X(t)$  is a multivariate white noise process its multivariate spectrum is given by  $S(f) = \Delta\Gamma$ , where  $\Gamma$  is the covariance matrix of  $X(t)$ . For the multitaper multivariate spectrum estimator to be unbiased for multivariate white noise we require  $E\{\hat{S}(f)\} = \Delta\Gamma$ , but in this case

$$E\{\hat{S}(f)\} = \int_{-f_N}^{f_N} U(f - f')S(f') df' = \Delta\Gamma \int_{-f_N}^{f_N} U(f - f') df',$$

and since, by taper property (ii),  $U(f)$  is periodic, the requirement is that

$$\int_{-f_N}^{f_N} U(f) df = \frac{1}{K\Delta} \sum_{k=0}^{K-1} \gamma_k \int_{-f_N}^{f_N} |U_k(f)|^2 df = \frac{1}{K\Delta} \sum_{k=0}^{K-1} \gamma_k \Delta \sum_{t=1}^N u_k^2(t) = \frac{1}{K} \sum_{k=0}^{K-1} \gamma_k = 1.$$

Thus for unbiasedness in the multivariate white noise case we must have  $\sum \gamma_k = K$ . We shall require this, and since  $\lambda_k = \gamma_k/K$  we hence require  $\sum \lambda_k = 1$ . However,  $\sum \lambda_k = \text{tr}(Q)$ , where  $\text{tr}(Q)$  is the trace of  $Q$ , and hence our  $Q$  matrix must be scaled so that  $\text{tr}(Q) = 1$ . All our examples in § 4 satisfy this requirement.

However, by taper property (i),  $u_j(\cdot)$  and  $u_k(\cdot)$  are orthonormal, and, by property (ii),  $U_j(\cdot)$  and  $U_k(\cdot)$  are periodic with period  $1/\Delta$ , so the integral becomes

$$\int_{-f_N}^{f_N} U_j(f)U_k^H(f) df = \Delta^2 \sum_{t=1}^N \sum_{s=1}^N u_j(t)u_k(s) \int_{-f_N}^{f_N} e^{-i2\pi f(t-s)\Delta} df = \Delta \sum_{t=1}^N u_j(t)u_k(t) = \Delta\delta_{j,k}. \tag{9}$$

Setting  $j = k$  we see that the integral of  $|U_k(f)|^2$  is thus  $\Delta$ , which combined with the requirement that  $\sum \gamma_k = K$  means that  $U(f)$  in (8) integrates to unity, justifying the stated taper property (iv), since  $U(f)$  is clearly periodic with the same period as the  $|U_k(f)|$ .

For a fixed number  $K$  of tapers and for continuous spectra,  $\hat{S}(f)$  will be asymptotically unbiased if taper property (v) holds, that is each  $|U_k(f)|^2$  behaves like  $\Delta\delta(f)$ , where  $\delta(\cdot)$  is the Dirac delta, as  $N \rightarrow \infty$ . In § 4 asymptotic unbiasedness is shown to hold for all the multitaper estimators discussed.

The smoothing bias for a general element  $\hat{S}_{lm}(f)$  of the spectral matrix is defined as  $b_1(f) = E\{\hat{S}_{lm}(f)\} - S_{lm}(f)$ . Given taper property (iv) and the fact that  $S_{lm}(f)$  is clearly

periodic with period  $1/\Delta$ , we can follow the standard approach (Percival & Walden, 1993, p. 245) which assumes that  $S_{lm}(f)$  can be expanded in a Taylor series about  $f$ , to find that a good approximation to the bias is given by

$$b_1(f) \simeq \frac{S''_{lm}(f)}{2} \int_{-f_N}^{f_N} \phi^2 U(\phi) d\phi = \frac{S''_{lm}(f)}{2} \beta_1,$$

say, where  $S''_{lm}(f)$  is the second derivative of the cross-spectrum. The integral in this expression can be written

$$\begin{aligned} \beta_1 &= \frac{1}{K\Delta} \sum_{k=0}^{K-1} \gamma_k \int_{-f_N}^{f_N} \phi^2 |U_k(\phi)|^2 d\phi = \frac{\Delta}{K} \sum_{k=0}^{K-1} \gamma_k \sum_{l=1}^N \sum_{m=1}^N u_k(l) u_k(m) \int_{-f_N}^{f_N} \phi^2 e^{-i2\pi\phi(l-m)\Delta} d\phi \\ &= \frac{1}{K} \sum_{k=0}^{K-1} \gamma_k u_k^H R u_k, \end{aligned} \quad (10)$$

where the matrix  $R$  has  $(l, m)$ th element

$$R_{lm} = \begin{cases} 1/(12\Delta^2) & \text{if } l = m, \\ (-1)^{l-m}/\{2(\pi\Delta)^2(l-m)^2\} & \text{if } l \neq m. \end{cases} \quad (11)$$

The form of  $R$  follows from Riedel & Sidorenko (1995, Lemma 3.2). Hence the smoothing biases  $b_1(f)$  of different multitaper cross-spectrum estimators with different smoothing windows can be compared by computing the real, positive quantity  $\beta_1$  in (10).

Now write the cross-spectrum as  $S_{lm}(f) = |S_{lm}(f)| \exp\{i\theta_{lm}(f)\}$ , where  $|S_{lm}(f)|$  is the cross-amplitude spectrum and  $\theta_{lm}(f)$  is the phase spectrum. Similarly write  $\hat{S}_{lm}(f) = |\hat{S}_{lm}(f)| \exp\{i\hat{\theta}_{lm}(f)\}$ , with  $\hat{\theta}_{lm}(f) = \theta_{lm}(f) + \rho\theta_{lm}(f)$ , where  $\rho\theta_{lm}(f)$  is a small increment such that  $\cos\{\rho\theta_{lm}(f)\} \simeq 1$  and  $\sin\{\rho\theta_{lm}(f)\} \simeq \rho\theta_{lm}(f)$ . Then

$$\begin{aligned} E\{|\hat{S}_{lm}(f)|\} - |S_{lm}(f)| &\simeq \frac{\beta_1}{2} \left[ \frac{d^2}{df^2} |S_{lm}(f)| - |S_{lm}(f)| \left\{ \frac{d}{df} \theta_{lm}(f) \right\}^2 \right], \\ E\{i\hat{\theta}_{lm}(f)\} - \theta_{lm}(f) &\simeq \frac{\beta_1}{2} \left[ \left\{ \frac{d}{df} \theta_{lm}(f) \right\} \left\{ \frac{d}{df} \log |S_{lm}(f)|^2 \right\} + \frac{d^2}{df^2} \theta_{lm}(f) \right]. \end{aligned}$$

The second expression can also be found in Jenkins & Watts (1968, p. 400). For the bias in the estimator of the cross-amplitude spectrum, the second term on the right is the misalignment bias. The phase spectrum will be steeper the larger the time delay between  $X_l(t)$  and  $X_m(t)$ , and hence the bias can be minimised by aligning the series. Now the first derivative of the phase spectrum is likely to dominate the second derivative; for example, a pure delay relationship gives a straight line for the phase spectrum. Hence the bias in the estimator of the phase spectrum is likely to be large only when the derivative of  $\log |S_{lm}(f)|^2$  is large.

The smoothing bias compares the mean of the estimator with the exact value at a point frequency  $f$ , but, for spectra which vary rapidly and/or have a large dynamic range, a serious concern is leakage out of the main resolution bandwidth of  $U(f)$  to other parts of the cross-spectrum. We define a 'leakage' or 'broad-band' bias as

$$b_2(f; W) = \int_{-f_N}^{f-W} U(f-f') S_{lm}(f') df' + \int_{f+W}^{f_N} U(f-f') S_{lm}(f') df',$$

where  $f-W$  to  $f+W$  is the resolution band for  $U(f-f')$ . If we assume that

$|S_{lm}(f)| \leq |S_{lm}|_{\max} < \infty$  over  $-f_N \leq f \leq f_N$ , the complex quantity  $b_2(f; W)$  can be bounded:

$$\begin{aligned} |b_2(f; W)| &\leq \left| \int_{-f_N}^{f-W} U(f-f')S_{lm}(f') df' \right| + \left| \int_{f+W}^{f_N} U(f-f')S_{lm}(f') df' \right| \\ &\leq \int_{-f_N}^{f-W} U(f-f')|S_{lm}(f')| df' + \int_{f+W}^{f_N} U(f-f')|S_{lm}(f')| df' \\ &\leq |S_{lm}|_{\max} \left[ 1 - \int_{-W}^W U(f) df \right] = |S_{lm}|_{\max} \beta_2(W). \end{aligned}$$

However,

$$\begin{aligned} \beta_2(W) &= 1 - \frac{1}{K\Delta} \sum_{k=0}^{K-1} \gamma_k \int_{-W}^W |U_k(f)|^2 df \\ &= 1 - \frac{\Delta}{K} \sum_{k=0}^{K-1} \gamma_k \sum_{l=1}^N \sum_{m=1}^N u_k(l)u_k(m) \int_{-W}^W e^{-i2\pi f(l-m)\Delta} df \\ &= 1 - \frac{1}{K} \sum_{k=0}^{K-1} \gamma_k u_k^H P(W) u_k, \end{aligned} \tag{12}$$

where the  $(l, m)$ th element of the matrix  $P(W)$  is

$$P_{lm}(W) = \begin{cases} 2W\Delta & \text{if } l = m, \\ \sin\{2\pi W(m-l)\Delta\} / \{\pi(m-l)\} & \text{if } l \neq m. \end{cases} \tag{13}$$

Thus the leakage biases  $|b_2(f; W)|$  of different multitaper cross-spectrum estimators with different smoothing windows can be compared by computing the real, positive bounding constant  $\beta_2(W)$  in (12). For multivariate white noise we have  $b_2(f; W) = \Delta \Gamma_{lm} \beta_2(W)$ , that is, the leakage bias may be computed exactly.

### 3.2. Variance of estimator

Suppose we let  $J_{k;l}(f)$  denote the  $l$ th component of  $J_k(f)$ . Then the  $(l, m)$ th element of  $\hat{S}(f)$  is given by

$$\hat{S}_{lm}(f) = \frac{1}{K} \sum_{k=0}^{K-1} \gamma_k J_{k;l}(f) J_{k;m}^H(f),$$

and

$$\text{var}\{\hat{S}_{lm}(f)\} = \frac{1}{K^2} \sum_{j=0}^{K-1} \sum_{k=0}^{K-1} \gamma_j \gamma_k \text{cov}\{J_{j;l}(f) J_{j;m}^H(f), J_{k;l}(f) J_{k;m}^H(f)\}. \tag{14}$$

Suppose the  $J$ 's have a multivariate complex Gaussian distribution. For finite sample sizes this will be the case if  $X(t)$  is multivariate Gaussian. The complex version of the Isserlis theorem (Koopmans, 1974, p. 27) then gives

$$\begin{aligned} \text{cov}\{J_{j;l}(f) J_{j;m}^H(f), J_{k;l}(f) J_{k;m}^H(f)\} &= E\{J_{j;l}(f) J_{k;l}^H(f)\} E\{J_{j;m}^H(f) J_{k;m}(f)\} \\ &\quad + E\{J_{j;l}(f) J_{k;m}(f)\} E\{J_{j;m}^H(f) J_{k;l}^H(f)\}. \end{aligned} \tag{15}$$

From (7) we obtain

$$E\{J_{j;l}(f)J_{k;l}^H(f)\} = \frac{1}{\Delta} \int_{-f_N}^{f_N} U_j(f-f')U_k^H(f-f')S_{ll}(f')df'$$

The other expectation terms in (15) follow readily from (5). By taper property (vii),  $S(f)$  is essentially constant across the designed resolution bandwidth of all the  $U_k(\cdot)$ , so that

$$E\{J_{j;l}(f)J_{k;l}^H(f)\}E\{J_{j;m}^H(f)J_{k;m}(f)\} \simeq \frac{S_{ll}(f)S_{mm}(f)}{\Delta^2} \left| \int_{-f_N}^{f_N} U_j(f-f')U_k^H(f-f')df' \right|^2$$

Using (9) we thus obtain

$$E\{J_{j;l}(f)J_{k;l}^H(f)\}E\{J_{j;m}^H(f)J_{k;m}(f)\} \simeq S_{ll}(f)S_{mm}(f)\delta_{jk}. \quad (16)$$

Making use of taper property (iii), we find that

$$E\{J_{j;l}(f)J_{k;m}(f)\}E\{J_{j;m}^H(f)J_{k;l}^H(f)\} \simeq (-1)^{j+k} \frac{|S_{lm}(f)|^2}{\Delta^2} \left| \int_{-f_N}^{f_N} U_j(f+f')U_k(f-f')df' \right|^2. \quad (17)$$

Since, by taper property (ii),  $U_j(\cdot)$  and  $U_k(\cdot)$  are periodic functions with period  $1/\Delta$ , we have

$$\int_{-f_N}^{f_N} U_j(f+f')U_k(f-f')df' = \int_{-f_N}^{f_N} U_j(f')U_k(2f-f')df' = \Delta \sum_{t=1}^N u_j(t)u_k(t)e^{-i4\pi ft\Delta}.$$

If we let  $V_{j,k}(2f) = |\sum u_j(t)u_k(t) \exp(-i4\pi ft\Delta)|^2$  then (14), (16) and (17) give

$$\begin{aligned} \text{var}\{\hat{S}_{lm}(f)\} &\simeq \frac{1}{K^2} \sum_{j=0}^{K-1} \sum_{k=0}^{K-1} \gamma_j \gamma_k \{S_{ll}(f)S_{mm}(f)\delta_{j,k} + (-1)^{j+k}|S_{lm}(f)|^2 V_{j,k}(2f)\} \\ &= \frac{S_{ll}(f)S_{mm}(f)}{K^2} \sum_{k=0}^{K-1} \gamma_k^2 + \frac{|S_{lm}(f)|^2}{K^2} \sum_{j=0}^{K-1} \sum_{k=0}^{K-1} (-1)^{j+k} \gamma_j \gamma_k V_{j,k}(2f) \\ &= \frac{S_{ll}(f)S_{mm}(f)}{K^2} \sum_{k=0}^{K-1} \gamma_k^2 \\ &\quad + \frac{|S_{lm}(f)|^2}{K^2} \left\{ \sum_{k=0}^{K-1} \gamma_k^2 V_{k,k}(2f) + \sum_{j=0}^{K-1} \sum_{k \neq j}^{K-1} (-1)^{j+k} \gamma_j \gamma_k V_{j,k}(2f) \right\}. \end{aligned}$$

When  $f = 0, \pm f_N$ ,  $V_{k,k}(2f) = 1$  and  $V_{j,k}(2f) = 0$  ( $j \neq k$ ), since the tapers are orthonormal, and  $|S_{lm}(f)|^2 = S_{lm}^2(f)$ , as  $S_{lm}(f)$  is real. Hence,

$$\text{var}\{\hat{S}_{lm}(f)\} \simeq \{S_{ll}(f)S_{mm}(f) + S_{lm}^2(f)\} \sum_{k=0}^{K-1} \gamma_k^2 / K^2 \quad (f = 0, \pm f_N).$$

The expression for  $V_{j,k}(2f)$  was examined in Walden, McCoy & Percival (1994, p. 481). When  $W < |f| < f_N - W$ , the term  $\sum u_j(t)u_k(t) \exp(-i4\pi ft\Delta)$  does not overlap its conjugate, and hence  $V_{j,k}(2f)$  terms contribute negligibly. Thus,

$$\text{var}\{\hat{S}_{lm}(f)\} \simeq S_{ll}(f)S_{mm}(f) \sum_{k=0}^{K-1} \gamma_k^2 / K^2 \quad (W < |f| < f_N - W).$$

For unbiasedness for multivariate white noise, however, we require  $\sum \gamma_k = K$ , and hence,



if we define

$$n = \left( \sum_{k=0}^{K-1} \gamma_k \right)^2 / \sum_{k=0}^{K-1} \gamma_k^2, \tag{18}$$

we can write

$$\text{var}\{\hat{S}_{lm}(f)\} \simeq \begin{cases} S_{ll}(f)S_{mm}(f)/n & (W < |f| < f_N - W), \\ \{S_{ll}(f)S_{mm}(f) + S_{lm}^2(f)\}/n & (f = 0, \pm f_N). \end{cases} \tag{19}$$

This result illustrates the pivotal role played by the eigenvalues of  $Q$ : different ‘distributions’ of eigenvalues give rise to different values of  $n$ . Note that when  $l = m$  we get

$$\text{var}\{\hat{S}_{ll}(f)\} \simeq \begin{cases} S_{ll}^2(f)/n & (W < |f| < f_N - W), \\ 2S_{ll}^2(f)/n & (f = 0, \pm f_N). \end{cases}$$

### 3.3. Asymptotic distribution of spectrum estimator

In § 3.2 we derived second moment results by assuming  $X(t)$  to have an  $N$ -dimensional multivariate Gaussian distribution. Suppose now we assume that the number of tapers  $K$  is fixed, but let  $N \rightarrow \infty$ . From taper property (v), the resolution width decreases with increasing sample size; that is  $W \rightarrow 0$  as  $N \rightarrow \infty$ . We now define a mixing assumption (Brillinger, 1981, pp. 9, 26) on our multivariate process.

*Mixing Assumption.* We assume that  $X(t)$  is strictly stationary with components  $X_1(t), \dots, X_L(t)$ , all of whose moments exist and such that

$$\sum_{t_1, \dots, t_{j-1} = -\infty}^{\infty} |c_{a_1, \dots, a_j}(t_1, \dots, t_{j-1}, 0)| < \infty$$

for  $a_1, \dots, a_j = 1, \dots, L$  and  $j = 2, 3, \dots$ , with  $c_{a_1, \dots, a_j}(t_1, \dots, t_j)$  denoting the joint cumulant function of order  $j$ .

We note that in the multivariate Gaussian case the mixing assumption corresponds to our existing assumption that  $\sum_{\tau} |s_{lm}(\tau)| < \infty$  ( $l, m = 1, \dots, L$ ).

Under the Mixing Assumption and the assumption that taper property (vi) holds, it follows from Brillinger (1981, p. 235) that  $J_k(f)$  is distributed asymptotically as

$$J_k(f) \sim \begin{cases} \mathcal{N}_L^C\{0, S(f)\} & (f \neq 0, \pm f_N), \\ \mathcal{N}_L\{0, S(f)\} & (f = 0, \pm f_N), \end{cases}$$

where  $\mathcal{N}_L^C\{0, S(f)\}$  denotes the dimension- $L$  complex Gaussian distribution with mean zero and covariance matrix  $S(f)$ , and  $\mathcal{N}_L\{0, S(f)\}$  denotes the real equivalent. Moreover,  $J_k(f)J_k^H(f)$  is distributed asymptotically as

$$J_k(f)J_k^H(f) \sim \begin{cases} \mathcal{W}_L^C\{1, S(f)\} & (f \neq 0, \pm f_N), \\ \mathcal{W}_L\{1, S(f)\} & (f = 0, \pm f_N), \end{cases}$$

where  $\mathcal{W}_L^C\{1, S(f)\}$  denotes the dimension- $L$  complex Wishart distribution with one degree of freedom, and  $\mathcal{W}_L\{1, S(f)\}$  denotes the real equivalent (Brillinger, 1981, pp. 89–90).

Now let the  $L \times L$  matrix-valued complex random variable  $C^{(n)}(f)$  have the complex Wishart distribution with  $n$  degrees of freedom, that is  $C^{(n)}(f) \sim \mathcal{W}_L^C\{n, S(f)\}$ , and let the

$L \times L$  matrix-valued real random variable  $R^{(n)}(f)$  have the real Wishart distribution with  $n$  degrees of freedom, that is  $R^{(n)}(f) \sim \mathcal{W}_L^C\{n, S(f)\}$ . Then (Brillinger, 1981, p. 90)

$$E\{(1/n)C^{(n)}(f)\} = S(f), \quad \text{var}\{(1/n)C_{lm}^{(n)}\} = S_{ll}(f)S_{mm}(f)/n,$$

where  $C_{lm}^{(n)}$  denotes the  $(l, m)$ th element of  $C^{(n)}$ , and (Kendall, 1975, pp. 77–8)

$$E\{(1/n)R^{(n)}(f)\} = S(f), \quad \text{var}\{(1/n)R_{lm}^{(n)}\} = \{S_{ll}(f)S_{mm}(f) + S_{lm}^2(f)\}/n.$$

Hence  $\hat{S}(f)$  can be written as

$$\hat{S}(f) \equiv \begin{cases} (1/K) \sum_{k=0}^{K-1} \gamma_k C^{(1)}(f) & (f \neq 0, \pm f_N), \\ (1/K) \sum_{k=0}^{K-1} \gamma_k R^{(1)}(f) & (f = 0, \pm f_N). \end{cases}$$

The fact that  $E\{C^{(1)}(f)\} = E\{R^{(1)}(f)\} = S(f)$ , combined with  $\sum \gamma_k = K$ , means that  $E\{\hat{S}(f)\} = S(f)$ , so that asymptotic unbiasedness is assured.

Further, from Brillinger (1981, p. 519) we know that since the tapers are orthonormal then for  $f \neq 0, \pm f_N$  the  $J_k(f)$  ( $k = 0, \dots, K-1$ ) are asymptotically independent multivariate complex Gaussian, and hence the  $J_k(f)J_k^H(f)$  ( $k = 0, \dots, K-1$ ) are independently distributed, each with the complex Wishart distribution with one degree of freedom. For  $f = 0, \pm f_N$  the  $J_k(f)$  ( $k = 0, \dots, K-1$ ) are asymptotically independent multivariate Gaussian, and hence the  $J_k(f)J_k^H(f)$  ( $k = 0, \dots, K-1$ ) are independently distributed, each with the real Wishart distribution with one degree of freedom. Hence, asymptotically,

$$\text{var}\{\hat{S}_{lm}(f)\} = \begin{cases} S_{ll}(f)S_{mm}(f)/n & (f \neq 0, \pm f_N), \\ \{S_{ll}(f)S_{mm}(f) + S_{lm}^2(f)\}/n & (f = 0, \pm f_N). \end{cases} \quad (20)$$

Since  $W \rightarrow 0$  as  $N \rightarrow \infty$  we see that (19) and (20) agree asymptotically.

For independent  $C_k^{(1)} \sim \mathcal{W}_L^C\{1, S(f)\}$  ( $k = 0, \dots, K-1$ ) we know that

$$\frac{1}{K} \sum_{k=0}^{K-1} C_k^{(1)} \sim \frac{1}{K} \mathcal{W}_L^C\{K, S(f)\},$$

Brillinger (1981, pp. 89–90). An analogous result holds for the real Wishart distribution (Seber, 1984, p. 21). Hence, if  $\gamma_k = 1$  for  $k = 0, \dots, K-1$ , giving  $n = K$ , we have that asymptotically

$$\hat{S}(f) \sim \begin{cases} (1/n) \mathcal{W}_L^C\{n, S(f)\} & (f \neq 0, \pm f_N), \\ (1/n) \mathcal{W}_L^C\{n, S(f)\} & (f = 0, \pm f_N). \end{cases} \quad (21)$$

If  $\gamma_k \neq 1$  for  $k = 0, \dots, K-1$ , we can approximate the asymptotic distribution of  $\hat{S}(f)$  by (21), with  $n$  given by (18), which yields the correct mean and variance for  $\hat{S}(f)$ ; as a result we call  $n$  in (18) the equivalent degrees of freedom of the estimator.

#### 4. CLASSES OF ORTHOGONAL MULTITAPER ESTIMATORS

Here we show that a number of well-known cross-spectrum estimators can be readily written in the form (3). We justify taper property (v), and where appropriate (vi), and examine the asymptotic statistical properties of the estimators. We also compare their smoothing and leakage bias for fixed degrees of freedom  $n$ . Some additional illustrative figures can be found at <http://stats.ma.ic.ac.uk/~atw>.

4.2. Minimising leakage: Slepian tapers

Thomson (1982) and Walden (1991) used ‘Slepian’ multitapers in cross-spectrum estimation. The taper design concentrates on sidelobe suppression. The first of the sequences,  $\{u_0^{(S)}(t), t = 1, \dots, N\}$ , is chosen such that its corresponding spectral window  $|U_0(f)|^2$  maximises the concentration ratio over the chosen interval  $[-W^{(S)}, W^{(S)}]$  with design bandwidth  $2W^{(S)}$ :

$$\int_{-W^{(S)}}^{W^{(S)}} |U_0(f)|^2 df \Big/ \int_{-f_N}^{f_N} |U_0(f)|^2 df.$$

The second taper sequence,  $\{u_1^{(S)}(t), t = 1, \dots, N\}$ , is also chosen to maximise this concentration ratio, but subject to being orthogonal to the first. The third taper sequence similarly maximises the concentration ratio, but subject to being orthogonal to the first two, and so on. In fact the  $K$  taper sequences are merely the first  $K$  eigenvectors of  $P(W^{(S)})$  in (13); see for example Percival & Walden (1993, p. 104).

Maximisation of the concentration ratio ensures that the sidelobes are minimised in this sense. The ratio must be close to unity for  $\{u_k^{(S)}(t)\}$  to be a decent taper, but this holds only for the tapers of order  $k = 0, \dots, 2NW^{(S)}\Delta - 2$ , and hence this number  $K = 2NW^{(S)}\Delta - 1$  of tapers can be used.

The simple cross-spectrum estimator based on  $K$  Slepian tapers is of the form (3) with  $\gamma_k^{(S)} \equiv 1$  for  $k = 0, \dots, K - 1$ , so that  $h_k^{(S)} \equiv u_k^{(S)}$  ( $k = 0, \dots, K - 1$ ). The matrix  $Q = (1/K) \sum u_k^{(S)}(u_k^{(S)})^H$  is symmetric and  $KQ$  is idempotent. Since the first  $K = 2NW^{(S)}\Delta - 1$  eigenvalues of  $P(W^{(S)})$  are almost unity and the other  $N - K$  are almost zero, except typically one or two near the transition zone,  $KQ \approx P(W^{(S)})$ , and hence  $Q$  is close to Toeplitz.

By way of example, if we take  $N = 100$ ,  $\Delta = 1$  and ‘bandwidth-duration product’  $2NW^{(S)} = 6$ , where the resolution band is  $[-W^{(S)}, W^{(S)}] = [-0.03, 0.03]$  then we can use tapers of order  $k = 0, \dots, 4$ , that is  $K = 5$  tapers in total. Note that the associated number of complex degrees of freedom of the estimator at each frequency is  $K = 5 = n$ ; see (18).

If we turn to asymptotic properties, it was pointed out in § 3.1 that for a fixed number  $K$  of tapers, and continuous spectra,  $\hat{S}(f)$  will be asymptotically unbiased if taper property (v) holds; that is each  $|U_k(f)|^2$  behaves like  $\Delta\delta(f)$  as  $N \rightarrow \infty$ . For the Slepian tapers with  $K = 2NW^{(S)}\Delta - 1$  fixed, we know (Slepian, 1978, p. 1389) that, as  $N \rightarrow \infty$  and consequently  $W^{(S)} \rightarrow 0$ ,

$$\frac{\int_{-W^{(S)}}^{W^{(S)}} |U_k^{(S)}(f)|^2 df}{\int_{-f_N}^{f_N} |U_k^{(S)}(f)|^2 df} = \frac{1}{\Delta} \int_{-W^{(S)}}^{W^{(S)}} |U_k^{(S)}(f)|^2 df \rightarrow \Lambda_k(c),$$

with  $\Lambda_k(c)$  a constant depending on  $k$  and  $c$ , the latter depending only on the fixed product  $NW^{(S)}\Delta$ . Hence  $|U_k^{(S)}(f)|^2$ , for  $|f| \leq W^{(S)}$ , must grow as  $N \rightarrow \infty$  and  $W^{(S)} \rightarrow 0$ , and, since its integral over  $|f| \leq f_N$  is the constant  $\Delta$ ,  $|U_k^{(S)}(f)|^2$  indeed behaves like  $\Delta\delta(f)$  asymptotically (Jenkins & Watts, 1968, p. 31), and asymptotic unbiasedness follows. With regard to taper property (vi), the  $K$  discrete Slepian tapers correspond to sampling  $K$  rescaled, bounded taper functions, namely the prolate spheroidal wave functions, which are orthogonal over  $[-1, 1]$  for  $k = 0, \dots, K - 1$  (Slepian, 1978, p. 1389; Percival & Walden, 1993, p. 384). Hence under the mixing assumption on  $X(t)$  the asymptotic distributional and variance results of § 3.3 apply, including again asymptotic unbiasedness.

4.3. *Minimising smoothing bias: Sine tapers*

Just as the eigenvectors of  $P$  in (13), sorted by increasing order of the corresponding eigenvalues, give the Slepian tapers with increasing leakage, that is decreasing concentration, so the eigenvectors of  $R$  in (11), sorted by increasing order of the corresponding eigenvalues, give tapers with increasing smoothing bias. This class of tapers can be approximated by the simple sine tapers (Riedel & Sidorenko, 1995). The  $k$ th sine taper is given by

$$u_k^{(R)}(t) = \left( \frac{2}{N+1} \right)^{\frac{1}{2}} \sin \left\{ \frac{(k+1)\pi t}{N+1} \right\} \quad (t = 1, \dots, N).$$

The first term is a standardisation factor to ensure that these tapers are orthonormal. These tapers achieve a smaller local bias, that is the bias due to the smoothing by the main lobe of  $U(f)$ , than the Slepian tapers, at the expense of sidelobe suppression. Riedel & Sidorenko (1995) were able to show that the  $k$ th sinusoidal taper has its spectral energy concentrated in the frequency bands

$$\frac{k}{2(N+1)\Delta} \leq |f| \leq \frac{k+2}{2(N+1)\Delta} \quad (k = 0, \dots, N-1).$$

If  $K$  tapers are used we see that the resolution interval is given by  $[-W^{(R)}, W^{(R)}]$ , where  $W^{(R)} = (K+1)/\{2(N+1)\Delta\}$ .

The simple cross-spectrum estimator of the form (3) based on  $K$  sine tapers has  $\gamma_k^{(R)} \equiv 1$  for  $k = 0, \dots, K-1$ , so that  $h_k^{(R)} \equiv u_k^{(R)}$  ( $k = 0, \dots, K-1$ ). The matrix  $Q = (1/K) \sum u_k^{(R)}(u_k^{(R)})^T$  is symmetric, and  $KQ$  is idempotent. The eigenvalues of  $R$  are slowly varying, so that  $Q$  formed as above will not be closely proportional to the Toeplitz matrix  $R$ , and  $Q$  is indeed non-Toeplitz.

If we take  $N = 100$  and  $\Delta = 1$  then the use of  $K = 5$  sine tapers yields a multitaper estimator with  $W^{(R)} \equiv 6/\{2(N+1)\} \approx 0.03$ , so that the resolution band is  $[-W^{(R)}, W^{(R)}] = [-0.03, 0.03]$ , just as for the Slepian tapers example. The associated number of complex degrees of freedom of the estimator at each frequency is again  $K = 5 = n$ .

With regard to taper property (v), the quantity  $|U_k^{(R)}(f)|^2$  grows as  $\sqrt{N}$  for  $|f| = k/\{2(N+1)\}$  (Riedel & Sidorenko, 1995, p. 190), and since the latter tends to zero for any fixed  $k$  as  $N \rightarrow \infty$  and the integral of  $|U_k^{(R)}(f)|^2$  over  $|f| \leq f_N$  is again  $\Delta$ , because of the normalisation of the tapers,  $|U_k^{(R)}(f)|^2$  also behaves in the limit like  $\Delta\delta(f)$ . Asymptotic unbiasedness follows and  $W^{(R)} \rightarrow 0$  as  $N \rightarrow \infty$  for fixed  $K$ . With respect to taper property (vi), the  $K$  discrete sine tapers correspond to sampling  $K$  rescaled, bounded taper functions, namely the sine functions, which are of course orthogonal over  $[0, \pi]$  for  $k = 0, \dots, K-1$ . Hence under the mixing assumption on  $X(t)$  the asymptotic distributional and variance results of § 3.3 again apply, including asymptotic unbiasedness.

4.4. *Weighted overlapped segment averaged estimators*

Welch (1967) introduced the idea of spectrum estimation via tapering overlapping blocks of data, calculating the direct spectrum estimator of each block, and then averaging. This method is known as Welch's 'weighted overlapped segment averaging,' see for example Carter (1987), and extends readily to cross-spectrum estimation. The time series is divided into  $N_B$  blocks each of size  $N_S$ . An integer-valued shift of size  $q$  is applied between successive blocks, so that  $0 < q \leq N_S$  and  $q(N_B - 1) = N - N_S$ . Let  $g(1), \dots, g(N_S)$  be a standard data

taper, with  $\sum g^2(t) = 1$ . Welch's cross-spectrum estimator is defined by

$$\hat{S}_{lm}^{(W)}(f) \equiv \frac{1}{N_B} \sum_{b=0}^{N_B-1} \hat{S}_{lm;b}^{(W)}(f),$$

where the estimator for block  $b$  is

$$\hat{S}_{lm;b}^{(W)}(f) \equiv \Delta \left\{ \sum_{s=1}^{N_S} g(s) X_l(s + bq) e^{-i2\pi f s \Delta} \right\} \left\{ \sum_{t=1}^{N_S} g(t) X_m(t + bq) e^{i2\pi f t \Delta} \right\}.$$

The number of overlapping points in each block is  $N_S - q$ , so that  $q = N_S$  corresponds to no overlap. With these restrictions on  $q$ , the  $b = 0$  block for the  $l$ th process utilises the data values  $X_l(1), \dots, X_l(N_S)$ , while the final  $b = N_B - 1$  block uses  $X_l(N - N_S + 1), \dots, X_l(N)$ . As done by Bronez (1992) for Welch's spectra, we can rewrite the estimator for block  $b$  as

$$\hat{S}_{lm;b}^{(W)}(f) = \Delta \left\{ \sum_{s=1}^N g_b(s) X_l(s) e^{-i2\pi f s \Delta} \right\} \left\{ \sum_{t=1}^N g_b(t) X_m(t) e^{i2\pi f t \Delta} \right\},$$

where

$$g_b(t) = \begin{cases} g(t - bq) & \text{if } t = bq + 1, \dots, bq + N_S, \\ 0 & \text{otherwise.} \end{cases} \quad (22)$$

Hence

$$\hat{S}_{lm}^{(W)}(f) = \frac{\Delta}{N_B} \sum_{b=0}^{N_B-1} \left\{ \sum_{s=1}^N g_b(s) X_l(s) e^{-i2\pi f s \Delta} \right\} \left\{ \sum_{t=1}^N g_b(t) X_m(t) e^{i2\pi f t \Delta} \right\}, \quad (23)$$

so that the estimator appears to be of the form (4) with  $K = N_B$ . However, in (4) the tapers are orthogonal, while the tapers in (22) are certainly not orthogonal when there is overlap, that is  $q < N_S$ . In what follows we show that (23) can be rewritten in terms of orthogonal tapers. Write (23) as  $\hat{S}_{lm}^{(W)}(f) = \Delta Z_l^H B B^H Z_m$ , where  $B$  is an  $N \times N_B$  real matrix with  $b$ th column given by  $g_b(t)/N_B^{1/2}$  ( $t = 1, \dots, N$ ). The  $N \times N$  outer-product matrix  $B B^H$  is symmetric but non-Toeplitz, and is also positive definite since  $\hat{S}_{ll}^{(W)}(f) = \Delta Z_l^H B B^H Z_l \geq 0$ , because  $\hat{S}_{ll}^{(W)}(f)$  is made up of the sum of squared moduli. Hence,  $B B^H$  can be decomposed in the same way as  $Q$ . Thus,  $\hat{S}_{lm}^{(W)}(f)$  can be written as in (2), with  $\{\lambda_0^{(W)}, \dots, \lambda_{N-1}^{(W)}\}$  being the eigenvalues of  $B B^H$  and  $\{u_0^{(W)}, \dots, u_{N-1}^{(W)}\}$  the eigenvectors, normalised so that  $\|u_k^{(W)}\|^2 = 1$  ( $k = 0, \dots, N - 1$ ). The matrix  $B$  has as left-most column the scaled taper  $\{g(t)/N_B^{1/2}\}$  followed by zeros, and as right-most or  $N_B$ th column the same scaled taper preceded by zeros. If we assume that all the elements of  $\{g(t)\}$  are nonzero, the columns of  $B$  are linearly independent since the  $j$ th column consists of  $(j - 1)q$  zeros followed by  $g(t)$  followed by zeros, and hence no column can be constructed as a linear sum of other columns. Hence  $\text{rank}(B) = N_B$ . With  $\{g(t)\}$  real-valued we know from Seber (1984, p. 518) that  $\text{rank}(B) = \text{rank}(B^H B) = \text{rank}(B B^H)$  and hence  $\text{rank}(B B^H) = N_B$ .

The  $(i, j)$ th element of  $B B^H$  ( $1 \leq i, j \leq N$ ) is given by

$$(B B^H)_{ij} = \frac{1}{N_B} \sum_{l=1}^{N_B} g\{i - (l - 1)q\} g\{j - (l - 1)q\} 1\{(l - 1)q + 1 \leq i, j \leq (l - 1)q + N_S\}, \quad (24)$$

where  $1\{\cdot\}$  is the indicator function. As a result,

$$\begin{aligned}
\sum_{k=0}^{N-1} \lambda_k^{(W)} &= \text{tr}(BB^H) = \sum_{i=1}^N (BB^H)_{ii} \\
&= \sum_{l=1}^{N_B} \sum_{i=1}^N [g^2\{i - (l-1)q\}/N_B] 1\{(l-1)q + 1 \leq i \leq (l-1)q + N_S\} \\
&= \sum_{t=1}^{N_S} g^2(t) = 1,
\end{aligned}$$

as required.

Now  $\text{rank}(BB^H) = N_B$  so that  $\lambda_{N_B}^{(W)} = \dots = \lambda_{N-1}^{(W)} = 0$ , and if we define

$$\lambda_k^{(W)} \equiv \gamma_k^{(W)}/N_B \quad (k = 0, \dots, N_B - 1)$$

then Welch's cross-spectrum estimator  $\hat{S}_{lm}^{(W)}(f)$  can be written in the form of (3) with  $K = N_B$  and eigenvalues  $\gamma_k^{(W)}$  and eigenvectors  $u_k^{(W)}$ , for  $k = 0, \dots, N_B - 1$ . Similarly, Welch's cross-spectrum estimator can be written as an average of  $N_B$  direct cross-spectrum estimators, as in (4), using orthogonal data tapers

$$h_k^{(W)}(t) = u_k^{(W)}(t)(\gamma_k^{(W)})^{\frac{1}{2}} \quad (k = 0, \dots, N_B - 1).$$

A common recommendation in the engineering literature is to use a Hanning data taper defined by

$$g(t) = [2/\{3(N_S + 1)\}]^{\frac{1}{2}} [1 - \cos\{2\pi t/(N_S + 1)\}] \quad (t = 1, \dots, N_S)$$

on each block, with an overlap of approximately 50%. For  $N = 100$ , the choice of  $N_S = 32$  and  $q = 17$  gives  $N_B = 5$  blocks. The overlap is  $\frac{15}{32} = 47\%$ . From  $BB^H$  we obtain

$$\{\gamma_0^{(W)}, \dots, \gamma_4^{(W)}\} = \{1.255, 1.147, 1.0, 0.853, 0.745\};$$

note that  $\sum \gamma_k^{(W)} = 5 = N_B$ , or equivalently  $\sum \lambda_k^{(W)} = 1$ . The matrix  $BB^H$  has rank  $K = N_B = 5$ . For this set of  $\gamma_k^{(W)}$ , equation (18) gives the value 4.83, while from Percival & Walden (1993, eqn (294)), the number of complex degrees of freedom for Welch's spectrum estimator with overlap approximately 50% is  $n = 18N_B^2/(19N_B - 1) = 4.79$ , giving good agreement; note that  $n \simeq 5$ , the same  $n$  as for the earlier illustrative Slepian and sine tapers.

With regard to asymptotic properties for  $N_B$  fixed as  $N \rightarrow \infty$ , we note that  $N_S \rightarrow \infty$ , so that the spectral window corresponding to the standard data taper  $\{g(t), t = 1, \dots, N_S\}$  behaves like a delta function and  $\hat{S}_{lm}^{(W)}(f)$  will be asymptotically unbiased, and hence so will  $\hat{S}_{lm}^{(W)}(f)$  (Percival & Walden, 1993, p. 291). Given taper properties (i)–(iii) and (vii), if we assume  $X(t)$  is multivariate Gaussian, the variance approximation (19) applies. The asymptotic analytical form of these tapers, the eigenvectors of (24), is not known, so we cannot verify taper property (vi) and hence cannot formally claim that the results of § 3.3 are applicable to Welch's estimator. However computations indicate the eigenvectors converge to smooth bounded functions as  $N$  increases, at least when using the Hanning taper for  $\{g(t)\}$ .

#### 4.5. Lag window cross-spectrum estimators

The lag window cross-spectrum estimator incorporating a data taper,  $\{d(t)\}$ , takes the form

$$\hat{S}_{lm}^{(L)}(f) = \Delta \sum_{\tau=-(N-1)}^{N-1} w_p(\tau) \hat{s}_{lm}(\tau) e^{-i2\pi f\tau\Delta},$$

where

$$\hat{s}_{lm}(\tau) = \sum_{t=1}^{N-\tau} d(t+\tau)X_l(t+\tau)d(t)X_m(t) \quad (\tau \geq 0), \quad \hat{s}_{lm}(-\tau) \equiv \hat{s}_{ml}(\tau) \quad (\tau > 0).$$

Here  $\{w_p(\tau)\}$  is the lag window,  $p$  is the window parameter, the maximum lag, and  $w_p(\tau) = w_p(-\tau)$ . Hence we can write

$$\hat{S}_{lm}^{(L)}(f) = \Delta \sum_{s=1}^N \sum_{t=1}^N d(s)X_l(s)d(t)X_m(t)w_p(s-t)e^{-i2\pi f(s-t)\Delta} = \Delta Z_l^H Q Z_m,$$

where  $Q(s, t) = d(s)w_p(s-t)d(t)$ . A lag window spectrum estimator can sometimes be negative, and so  $Q$  need not be positive semidefinite in general. Percival & Walden (1993, p. 269) give an example where a Parzen lag window combined with a particular choice of nonrectangular taper can lead to a negative spectrum estimate. However, there are some popular practical cases where the estimator is nonnegative and  $Q$  will be positive semidefinite; the Parzen and ‘minimum-bias’ Papoulis lag windows combined with the default rectangular taper  $d(t) = 1/\sqrt{N}$  ( $t = 1, \dots, N$ ) are two such suitable choices, and both are defined in Percival & Walden (1993, pp. 265–6).

For these lag windows the number of complex degrees of freedom associated with the spectrum estimator is  $n = 1.85N/p$  for the Parzen and  $n = 1.7N/p$  for the Papoulis lag windows. Both have a similar shape. For the reduced-rank multitaper cross-spectrum estimators of §§ 4.2–4.4 the number of complex degrees of freedom is  $n = K$ , which is also the rank of  $Q$ . Hence, we might expect that, for the lag window case,  $n$  should be approximately equal to the rank of  $Q$ . The singular values of

$$Q(s, t) = d(s)w_p(s-t)d(t) = (1/N)w_p(s-t),$$

a Toeplitz matrix formed from the Parzen or Papoulis lag windows and default rectangular taper, guaranteed positive semidefinite, were calculated for  $N = 100$  and  $p$  chosen so that  $n = 5$  and 10, that is  $p = 37$  and 19, respectively. Note that

$$\sum \lambda_k = \text{tr}(Q) = N\{(1/N)w_p(0)\} = w_p(0) = 1,$$

as required. The results for Parzen and Papoulis lag windows were very similar; henceforth we only discuss the Parzen case. When  $n = 5$ , the first five singular values contribute over 90% of the total of unity, while when  $n = 10$  the first ten singular values explain over 92% of the total. Hence, the value of  $n$  is reasonably good at predicting the ‘effective’ rank of  $Q$ , but is an underestimate. The problem is of course that these lag window estimators actually correspond to full-rank  $Q$  matrices.

A positive semidefinite lag window cross-spectrum estimator can be written as in (2), with eigenvalues of  $Q$ ,  $\{\lambda_0^{(L)}, \dots, \lambda_{N-1}^{(L)}\}$ ,  $\sum_k \lambda_k^{(L)} = 1$ , and eigenvectors  $\{u_0^{(L)}, \dots, u_{N-1}^{(L)}\}$ , normalised so that  $\|u_k^{(L)}\|^2 = 1$  ( $k = 0, \dots, N-1$ ). Define  $n_B$  as an integer satisfying  $n < n_B \ll N$  such that  $\lambda_{n_B}^{(L)} \approx \dots \approx \lambda_{N-1}^{(L)} \approx 0$ . Then the lag-window cross-spectrum estimator can be written approximately as an average of  $n_B$  direct cross-spectrum estimators, using the orthogonal data tapers  $h_k^{(L)}(t) = u_k^{(L)}(t)(\gamma_k^{(L)})^{\frac{1}{2}}$  ( $k = 0, \dots, n_B - 1$ ):

$$\begin{aligned} \hat{S}_{lm}^{(L)}(f) &\approx \frac{\Delta}{n_B} \sum_{k=0}^{n_B-1} \gamma_k^{(L)} \left\{ \sum_{s=1}^N u_k^{(L)}(s)X_l(s)e^{-i2\pi fs\Delta} \right\} \left\{ \sum_{t=1}^N u_k^{(L)}(t)X_m(t)e^{i2\pi ft\Delta} \right\} \\ &= \frac{\Delta}{n_B} \sum_{k=0}^{n_B-1} \left\{ \sum_{s=1}^N h_k^{(L)}(s)X_l(s)e^{-2\pi fs\Delta} \right\} \left\{ \sum_{t=1}^N h_k^{(L)}(t)X_m(t)e^{i2\pi ft\Delta} \right\}, \end{aligned} \quad (25)$$

where  $\lambda_k^{(L)} \equiv \gamma_k/n_B$  ( $k=0, \dots, n_B-1$ ). For example, for the Parzen lag window, with  $N=100$  and  $p=37$  for which  $n=5$ , the choice of  $n_B=8$  is such that

$$\lambda_0^{(L)} + \dots + \lambda_{n_B-1}^{(L)} > 0.99$$

and

$$\{\gamma_0^{(L)}, \dots, \gamma_7^{(L)}\} = \{2.123, 1.854, 1.476, 1.067, 0.696, 0.406, 0.209, 0.094\},$$

so that  $\gamma_0^{(L)} + \dots + \gamma_7^{(L)} = 7.925 \approx 8 = n_B$ . If we choose  $n_B=16$ , then

$$\lambda_0^{(L)} + \dots + \lambda_{15}^{(L)} > 0.999, \quad \gamma_0^{(L)} + \dots + \gamma_{15}^{(L)} = 15.986 \approx 16 = n_B.$$

In our example we chose the maximum lag  $p=37$  by using the standard effective complex degrees of freedom formula  $n=1.85N/p$  for the Parzen lag window (Percival & Walden, 1993, p. 269) and choosing  $n=5$ . However, as we now have the values  $\gamma_k$  we can also calculate  $n$  via (18); this gives  $n=5.3$  for  $n_B=8$  or  $16$ , so that reasonable agreement is achieved.

One form of lag window cross-spectrum estimator for which  $Q$  has reduced rank is the frequency-averaged cross-periodogram. Here the raw cross-periodograms are smoothed over  $K=2M+1$  adjacent Fourier frequencies, that is

$$\bar{S}_{lm}(f_i) = \frac{1}{K} \sum_{j=-M}^M \hat{S}_{lm}^{(P)}(f_{i-j}),$$

where  $f_i = i/(N\Delta)$  and the raw cross-periodogram is

$$\hat{S}_{lm}^{(P)}(f) = \Delta \left\{ \sum_{s=1}^N \frac{1}{\sqrt{N}} X_l(s) e^{-i2\pi f s \Delta} \right\} \left\{ \sum_{t=1}^N \frac{1}{\sqrt{N}} X_m(t) e^{i2\pi f t \Delta} \right\}.$$

For the estimator  $\bar{S}_{lm}(f_i)$  we obtain the symmetric Toeplitz matrix

$$Q(s, t) = (1/N)w(s-t) = \sin\{K\pi(s-t)/N\}/[NK \sin\{\pi(s-t)/N\}].$$

Since  $Q(s, t)$  can be written as a sum of  $K$  complex exponentials, that is

$$Q(s, t) = \frac{1}{NK} \sum_{j=-M}^M e^{i2\pi(s-t)j/N},$$

the symmetric degenerate matrix  $Q$  has rank  $K$  and its eigenvalues satisfy

$$\sum \lambda_k^{(P)} = \text{tr}(Q) = N\{(1/N)w(0)\} = w(0) = 1.$$

For example, if we take  $N=100$  and  $K=5$  we find that this matrix has rank 5 with  $\lambda_0^{(P)} = \dots = \lambda_4^{(P)} = 0.2$ . Note that  $\gamma_k^{(P)} \equiv K\lambda_k^{(P)} = 1$  for  $k=0, \dots, K-1$ . Hence  $\bar{S}_{lm}(f_i)$  may be written as in (4), with  $K=n_B=5$  and using the orthogonal data tapers  $h_k^{(L)}$  for  $k=0, \dots, K-1$ . For this estimator the effective half-bandwidth is  $W^{(L)} = K/(2N)$ .

The asymptotic properties of the frequency averaged cross-periodogram are well known. For fixed  $K=2M+1$ , the estimator  $\bar{S}_{lm}(f)$  at a fixed frequency  $f$  is asymptotically unbiased (Brillinger, 1981, Corollary 7.3.1). Furthermore, under the mixing assumption,  $\bar{S}(f)$  has, as would be expected, the asymptotic distribution specified by (21) (Brillinger, 1981, Theorem 7.3.3) with  $n=K$ .

#### 4.6. Comparison of spectral windows

The overall spectral windows given by (8) for our example cases with  $\Delta=1$  are shown in Fig. 1 on a decibel scale. While the frequency-averaged cross-periodogram has a



‘blocky’-type main lobe similar in shape to that of the Slepian or sine taper estimators, its poorer sidelobe behaviour is quite evident. The Welch and Parzen lag window estimators have less blocky spectral windows; the Welch estimator has a wide main lobe but low sidelobes, whereas the spectral window of lag window estimators has a characteristic very slow decay because the spectral window for the lag window estimator is the convolution of the smoothing window, that is the Fourier transform of  $w_p(\tau)$ , and Fejér’s kernel, and the slow decay of the latter predominates (Percival & Walden, 1993, § 6.11).

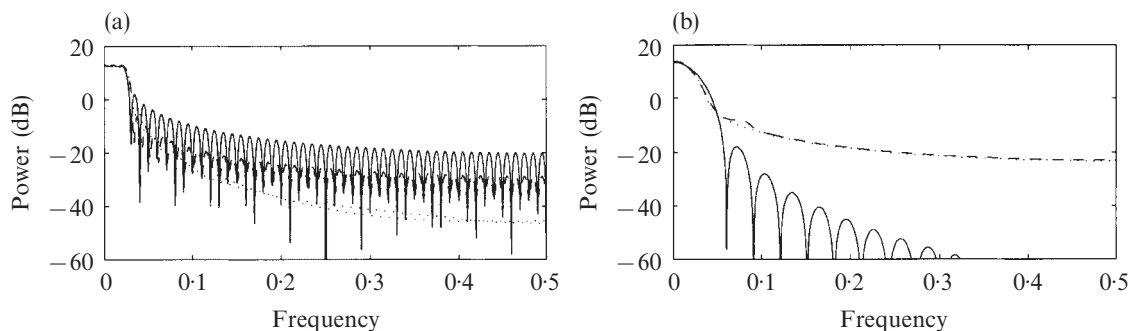


Fig. 1. Overall spectral windows on decibel (dB) scale. (a) Frequency-averaged cross-periodogram (solid line), sine tapers (dotted) and Slepian tapers (dashed). (b) Welch (solid line), lag window,  $n_B = 8$  (dotted) and  $n_B = 16$  (dashed). Each of the estimators has approximately 5 complex degrees of freedom.

#### 4.7. Comparison of leakage biases

The positive bounding constant  $\beta_2(W)$  in the leakage bias formula (12) can be written as unity minus a ‘concentration factor,’ where the concentration factor is  $(1/K) \sum \gamma_k u_k^H P(W) u_k$ . The concentration factor is plotted as a function of  $W$  for the five estimation classes in Fig. 2. As expected, the Slepian tapers method rapidly approaches unity around  $W = 0.03$ , the nominal value of the half-bandwidth which was used; recall that  $2W^{(S)}$  was chosen to be 0.06. The sine tapers do nearly as well, while Welch’s method gives a slower approach to unity. The frequency-averaged cross-periodogram and Parzen lag window method with  $n_B = 8$  and  $n_B = 16$  approach unity most slowly and have very poor leakage properties; this is not surprising in view of the weighting given to the ends

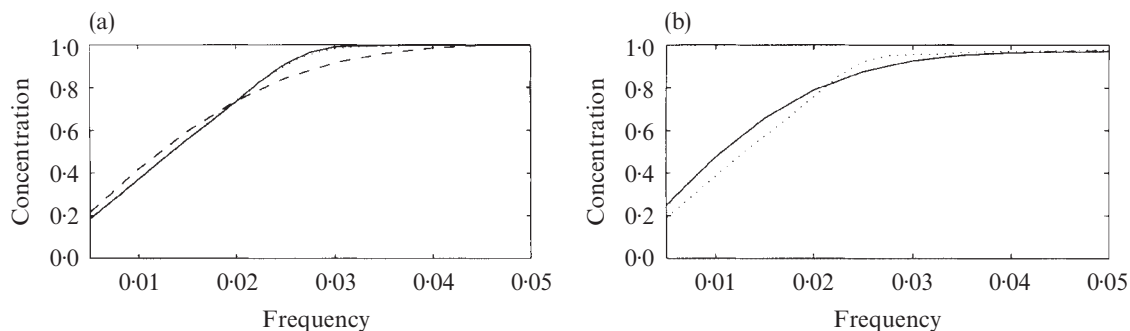


Fig. 2. Spectral concentration factor as a function of  $W$ . (a) Slepian tapers (solid line), sine tapers (dotted) and Welch (dashed). (b) Lag window,  $n_B = 8$  (solid line),  $n_B = 16$  (dashed) and frequency-average cross-periodogram (dotted).

of the data by the equivalent orthogonal tapers for these methods as shown at <http://stats.ma.ic.ac.uk/~atw>. The practical importance of poor lag window leakage is illustrated in § 5.

#### 4.8. Comparison of smoothing biases

The classes of orthogonal multitaper estimators discussed in §§ 4.2–4.5 are compared in terms of exact smoothing bias factors  $\beta_1$ , equation (10), in Table 1 for  $\Delta = 1$ . The results in Table 1 are for  $N = 100$  with the parameters chosen as explained previously to give estimators with  $n = 5$  complex degrees of freedom. Given the true cross-spectral matrix a fixed  $n$  effectively fixes the variance; see (19) and (20). The sine tapers, approximations to tapers which minimise smoothing bias, unsurprisingly have the lowest smoothing bias. The Slepian tapers, designed to minimise leakage bias, do less well, but still give much better results than the lag window classes.

Table 1. Smoothing bias factors  $\beta_1$ , equation (10), for different estimators with 5 complex degrees of freedom

Estimation class	Exact $\beta_1 \times 10^4$	Approximate $\beta_1 \times 10^4$
Sine tapers	2.71	2.94
Welch	3.06	—
Slepian tapers	3.51	3.00
Frequency-averaged cross-periodogram	9.01	3.00
Parzen lag window	9.02	—

For the estimators with an almost rectangular main lobe to the spectral window, that is Slepian tapers, sine tapers and the frequency averaged cross-periodogram, it is possible to derive approximate analytic expressions for  $\beta_1$ , also shown in Table 1. For  $\Delta = 1$  we know that  $\beta_1 = \int_{-1/2}^{1/2} \phi^2 U(\phi) d\phi$ , and if  $U(\cdot)$  is rectangular and integrates approximately to unity over the resolution band  $|f| \leq W$ , then

$$U(\phi) \simeq \begin{cases} 1/(2W) & \text{if } |\phi| \leq W, \\ 0 & \text{otherwise.} \end{cases} \quad (26)$$

As a result we get  $\beta_1 \simeq W^2/3$ , as in Thomson (1982, p. 1062). Hence, for our Slepian tapers example,  $W^{(S)} = 0.03$  and  $\beta_1 \simeq 3.0 \times 10^{-4}$ . For the sine tapers example  $W^{(R)} = (K+1)/\{2(N+1)\} = 0.0297$ , so that  $\beta_1 \simeq 2.94 \times 10^{-4}$ , while for our frequency averaged cross-periodogram example  $W^{(L)} = (K+1)/(2N) = 0.03$  and hence  $\beta_1 \simeq 3.0 \times 10^{-4}$ . While the approximations for Slepian and sine tapers are useful, because of the small leakage, that for the frequency averaged cross-periodogram is very poor; this is a result of the severe leakage for this estimator which means that the approximation in (26) is too inaccurate. Asymptotically, for Slepian and sine tapers,  $W \simeq K/(2N)$  so that for  $f \neq 0, \pm f_N$  it follows from (20) with  $n = K$  that the mean squared error is given by

$$\begin{aligned} E\{|\hat{S}_{lm}(f) - S_{lm}(f)|^2\} &= |\text{bias}\{\hat{S}_{lm}(f)\}|^2 + \text{var}\{\hat{S}_{lm}(f)\} \\ &= |S''_{lm}(f)|^2 \frac{\beta_1^2}{4} + \frac{1}{K} S_{ll}(f) S_{mm}(f) \\ &= |S''_{lm}(f)|^2 \left[ \frac{K^2}{24N^2} \right]^2 + \frac{1}{K} S_{ll}(f) S_{mm}(f), \end{aligned}$$

so that the mean squared error is minimised for  $K = \{144S_{ii}(f)S_{mm}(f)N^4/|S''_{lm}(f)|^2\}^{1/5}$ ; when the spectrum is rapidly varying the denominator will be large, reducing the nominal choice, and causing practitioners to use many fewer than  $K \propto N^{4/5}$  tapers.

4.9. Consistency in mean square

The estimator  $\hat{S}(f)$  is consistent in mean square if  $\lim_{N \rightarrow \infty} E\{|\hat{S}(f) - S(f)|^2\} = 0$ . For both Slepian and sine tapers, if we let  $K \rightarrow \infty$  such that  $K/N \rightarrow 0$  as  $N \rightarrow \infty$  then  $W^{(S)}$  and  $W^{(R)} \rightarrow 0$  as  $N \rightarrow \infty$ , since

$$W^{(S)} = (K + 1)/(2N\Delta), \quad W^{(R)} = (K + 1)/\{2(N + 1)\Delta\}.$$

Hence asymptotic unbiasedness is preserved, and since  $n = K$  for both estimators it follows from (19) and (20) that  $\text{var}\{\hat{S}(f)\} \rightarrow 0$  as  $N \rightarrow \infty$ , ensuring mean square consistency. For Welch's estimator, we let  $N_B \rightarrow \infty$  such that  $N_B/N \rightarrow 0$  and  $N_S \rightarrow \infty$  such that  $N_S/N \rightarrow 1$ , as  $N \rightarrow \infty$ . Asymptotic unbiasedness is thus retained. For Welch's method we showed in § 4.4 that the variance formula (19) applied when  $X(t)$  is multivariate Gaussian, and since  $n \propto N_B$  for an overlap of approximately 50% for large  $N_S$  (Percival & Walden, 1993, eqn (294)), mean square consistency follows in at least this case. Mean square consistency of lag window estimators is discussed in Priestley (1981, p. 464) who shows that we require  $p \rightarrow \infty$  while  $p/N \rightarrow 0$  as  $N \rightarrow \infty$ , or equivalently  $n \propto N/p \rightarrow \infty$  while  $n/N \rightarrow 0$  as  $N \rightarrow \infty$ . The frequency-averaged periodogram was analysed in Brillinger (1981) from which  $K \rightarrow \infty$  such that  $K/N \rightarrow 0$  as  $N \rightarrow \infty$ . The unifying requirement is that the number of complex degrees of freedom,  $n$ , or equivalently the bandwidth-duration product  $2WN$ , tends to infinity such that  $W \rightarrow 0$  as  $N \rightarrow \infty$ .

5. INVERTING ESTIMATED CROSS-SPECTRAL MATRICES

In carrying out a spectrum analysis of a set of  $L$  real-valued stationary processes it is often the case that it is not the cross-spectrum matrix itself which is of primary interest, but rather quantities derived from it. Perhaps the most useful is the fraction of power in the  $j$ th time series  $\{X_j(t)\}$ , at a frequency  $f$ , which can be linearly predicted from the other  $L - 1$  series, the so-called magnitude squared multiple coherence, denoted here by  $C_j^2(f)$ . It is a widely used scientific quantity (Foster & Guinzy, 1967; Carter, 1987; Kuo, Lindberg & Thomson, 1990; White, 1984; Percival, 1994; Walden & White, 1998) because of the insights it provides into the relationships between the series in different frequency ranges.

The multiple coherence of series  $j$  is given by  $C_j^2(f) = 1 - \{S_{jj}(f)S^{jj}(f)\}^{-1}$  (Jenkins & Watts, 1968, p. 487), where  $S^{jj}(f)$  is the  $j$ th diagonal element of the inverse of the full  $L \times L$  true cross-spectral matrix,  $S(f)$ . Note that to compute the multiple coherence it is necessary to construct the full cross-spectral matrix, invert it and then pick off the appropriate diagonal element. This must be done for all the frequencies of interest.

Hence, we need both to be able to estimate the elements of the cross-spectral matrix and also to invert it. Using the representation (6) for the estimated cross-spectral matrix we note that if  $K < L$  then  $L - K$  orthogonal vectors can be found that span the complement of the space spanned by the  $J_k(f)$  ( $k = 0, \dots, K - 1$ ). Since these vectors annihilate  $\hat{S}(f)$ , this matrix is of rank  $K$  or less. Thus a necessary condition for invertibility of the estimated cross-spectral matrix is that  $K \geq L$ . For Slepian or sine tapers  $K$  is the number of tapers, for Welch's parameterisation  $K = N_B$ , for the frequency-averaged cross-periodogram  $K$  is the number of frequencies averaged over, and for the Parzen or similar lag windows, if we choose  $n > L$ ,

then since  $n_B > n$  we have  $n_B > n > L$ , and the condition is satisfied. In all practical cases examined, the requirement  $K \geq L$  has resulted in an invertible matrix.

### 6. A PRACTICAL COMPARISON

Since the various methods examined here are all cast into the multitaper formulation, it might be felt that the difference displayed in for example Figs 1 and 2 are not important in practice. With a slowly-varying featureless spectrum this might well be true, but for a rapidly-varying spectrum with high dynamic range, as is commonly met in the physical sciences, different estimators perform very differently. To illustrate this, we consider a set of 60 contiguous seismic time series, with  $\Delta = 0.004$  seconds so that the Nyquist frequency is 125 Hz. All the series were subject to the same source and recording characteristics which decay rapidly around 4 Hz such that we would expect virtually zero coherent signal below 4 Hz (Walden, 1991) across all 60 series. Each series is of length  $N = 401$  points. Slepian multitaper and Papoulis lag window estimators were designed to have the same bandwidth and almost equal complex degrees of freedom, 11 and 12 respectively. The series were grouped into adjacent sets of  $L = 4$  series, a choice such that  $K > L$ , and which ensures alignment of the series in the groups of size  $L$ . Estimates  $\hat{C}_j^2(f)$  ( $j = 1, \dots, 4$ ) of multiple coherence at frequencies  $f = 1.95$  Hz and 3.9 Hz were computed from the first four series, the next four series, and so on, until all sixty series had been used, and these were binned into coherence ranges of width 0.1. With ideal estimation all the coherences estimated at 1.95 Hz should be zero, while all the coherences estimated at 3.9 Hz, near

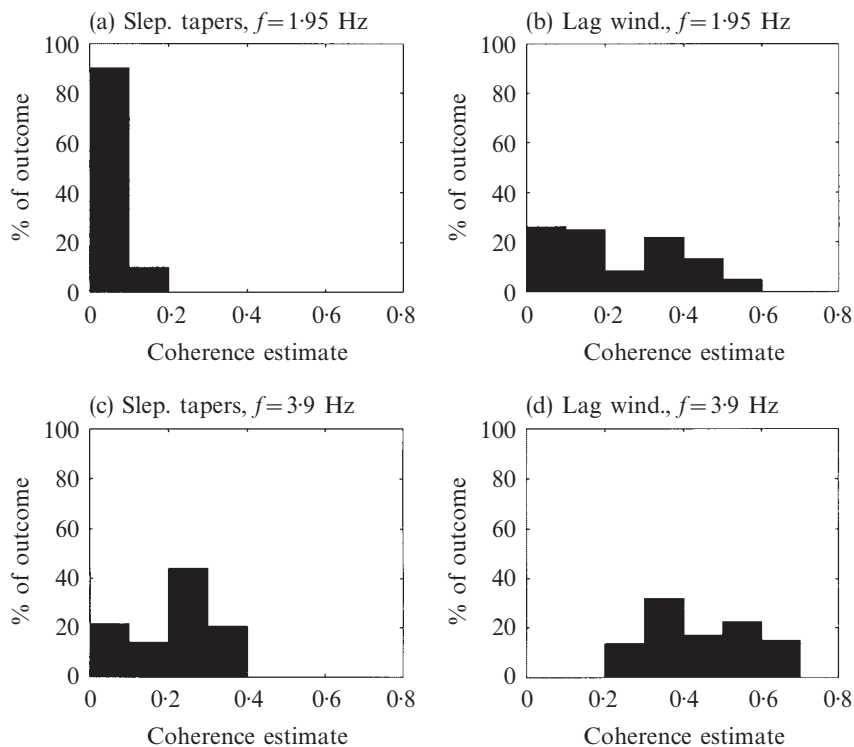


Fig. 3. Histograms of coherence results from 60 series at frequency 1.95 Hz using (a) Slepian tapers and (b) lag windowing, and at frequency 3.9 Hz using (c) Slepian tapers and (d) lag windowing.

the transition zone, should be nearly zero. The results are shown in Fig. 3. The top plots compare the histogram, in terms of the percentage of the 60 outcomes in each bin, of estimated coherence at  $f = 1.95$  Hz using (a) Slepian multitapers and (b) lag windowing, and the bottom plots (c) and (d) show the same for 3.9 Hz. We see that at  $f = 1.95$  Hz the Slepian multitapers method gives rise to very low estimated coherences, with nothing in excess of 0.2, while the lag window method has coherences spread out up to 0.6. For  $f = 3.9$  Hz the Slepian multitapers give estimated coherences between 0 and 0.4, with a peak centred on 0.25, while the lag window method has coherences spread out between 0.2 and 0.7. Since the physics tells us that we should expect zero coherence at 1.95 Hz and a very low coherence at 3.9 Hz, we see that the Slepian multitaper method has performed much better than the lag window approach; the greater leakage bias of the latter has proved its undoing here because of the large change in spectral power between frequencies less than 4 Hz and those above. In fact at other frequencies where there is no locally rapid change in spectral power the two approaches produce nearly identical results.

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