Spectral Estimation using the Multiple-Taper Method

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Abstract

A description of the multiple-taper method for spectral estimation and harmonic analysis is given. This method is particularly suitable for time series of short duration. Cross-spectral analysis using the multiple-taper method is treated and the jackknife method used to obtain confidence limits for spectra, coherences, and frequencies of harmonic components. A program written to implement the multiple-taper method is described.

1 Background

This report describes one of the latest methods developed for spectral estimation and time series analysis. It is not yet widely used, in part because it is still under development and the tendency of researchers to use "standard" tools when analysing their data. Also, this method is not incorporated in commercially available software packages for time series analysis. Its features seem, however, promising enough to encourage the development of the necessary software.

My work in the area of spectral analysis started in late 1992 when I was working for Sigfús J. Johnsen at the Geophysics Laboratory in Copenhagen. Sigfús's interest in the method presented here had been aroused by his French colleagues, who were analysing data from the Vostok ice-core (Yiou *et al.*, 1991). When I returned to Iceland, analysis of total ozone data from Reykjavík resumed. Previous studies had concentrated on parametric modelling of the data (Bjarnason *et al.*, 1992; Bjarnason *et al.*, 1993). The Dobson network of total ozone spectrophotometers has only been operating for roughly three decades, or since the international geophysics year in 1957. Therefore, time series of total ozone are typically quite short after the necessary averaging has been done (usually on a

monthly basis). Also, the data are often discontinuous, especially at high latitudes where measuring during the wintertime is difficult. This situation has put the main emphasis in analysis of ozone data on parametric modelling to determine trends and the influences of natural variations (e.g. the quasi biennial oscillation in equatorial zonal winds and the 11 year solar cycle) on total ozone. Spectral analysis of ozone and related data is on the other hand very limited (see Zerefos *et al.* 1992; Salby & Shea, 1991). The method described below seems quite adequate to expand the analysis of the ozone data into the frequency domain. The results of this analysis will be reported elsewhere (Rögnvaldsson & Bjarnason, 1993). We have also applied the multiple-taper method to analyze ice-core data from Greenland, quantum oscillations in the properties of metals (the de Haas–van Alphen effect), and time series of characteristics of a ferro-alloy plant.

2 Introduction

The aim of this paper is to give a short (and hopefully comprehensive) overview of the multiple-taper method for spectral estimation. The basis for the multiple-taper method (MTM) was first given by Thomson (1982). It has proved to be a powerful tool in spectral estimation (see, e.g. Kuo *et al.*, 1990; Park *et al.*, 1987; Lindberg & Park, 1987; Thomson, 1990a; Thomson 1990b; Yiou *et al.*, 1991), especially for the analysis of short time series. By a short time series we mean that the data can not be split up into independent series.

Section 3 is a brief overview of the properties of stationary processes and the fundamentals of spectrum estimation. Section 4 describes the basic structure of the MTM and estimation of power spectral density. In section 5, harmonic analysis and the estimation of statistical significance of harmonic components is treated. Finally, the last section comments on cross-spectral analysis with the MTM, regarding both coherence and phase. Appendix A is a detailed description of the program written in connection with this work and problems related to coding of the MTM. Appendix B gives a brief description of the jackknifing method for inferring a sample's statistical properties without the use of explicit probability distributions and comments are given on various statistical terms.

3 Spectral analysis

It is well known that almost all periodic functions can be represented as Fourier series, and non-periodic, absolutly integrable functions as Fourier integrals (Priestley, 1981). Functions in these classes can thus be thought of as sums, or integrals, of sin- and cosine components and it is natural to think of each frequency interval $(f, f + \mathrm{d}f)$ as contributing a small fraction to the total "power" or "energy".

Consider an absolutly integrable function $X(t) \in L^1(-\infty, \infty)$, i.e.

$$\int_{-\infty}^{\infty} |X(t)| \mathrm{d}t < \infty. \tag{1}$$

The total energy is then defined as

$$\int_{-\infty}^{\infty} X^2(t) \mathrm{d}t \tag{2}$$

and is finite. Hence, the spectral properties of $X(t)$ are described in terms of its energy density distribution. The contribution to the total energy of components with frequencies between f and $f + \mathrm{d}f$ is $|G(f)|^2 \mathrm{d}f$ where $G(f)$ is the Fourier transform of $X(t)$,

$$G(f) = \int_{-\infty}^{\infty} X(t) \exp(-i2\pi f t) \mathrm{d}t. \tag{3}$$

In the case of periodic functions the total energy is infinite and the spectral properties are described in terms of the distribution of power (i.e. energy per unit time) defined by

$$\lim_{T \to \infty} \frac{\int_{-T}^{T} X^2(t) \mathrm{d}t}{2T}. \tag{4}$$

The contribution to total power of each of the discrete frequency components is given by the square of the corresponding amplitude.

When analysing a stationary random process, an infinite number of realizations is possible. The spectral properties are thus only meaningful in the average sense. A further complication is that stationary random processes are neither periodic nor absolutly integrable. Hence, the above representation does not encompass these "functions" and the more general Cramér representation is needed.

In what followes we shall be considering a time series $x(t)$ and N contiguous observations of it, $x(0), x(1), \ldots, x(N-1)$, spaced at unit time intervals. Frequency in the spectral representation lies in the range $(-\frac{1}{2}, \frac{1}{2}]$ and angular frequency $\omega = 2\pi f \in (-\pi, \pi]$. Since we shall only be dealing with real processes later on, the actual range of f will be $[0, \frac{1}{2}]$ with the negative part of the spectrum given by the complex conjugate of its positive part.

Initially, we assume that the random process under study is wide sense stationary, i.e. its statistics are invariant under changes of time origin. In theoretical variance calculations it is also assumed that the process is Gaussian in the frequency domain, so that estimates of power spectra are the sums of squares of normally distributed variates and hence distributed as χ^2 (Thomson & Chave, 1990, give the probability density function of such a spectrum estimate). The spectral (or Cramér) representation of a stationary process is given by a generalized Fourier transform,

$$x(t) = \int_{-1/2}^{1/2} \exp(i2\pi f t) \mathrm{d}Z(f), \tag{5}$$

for all t where $\mathrm{d}Z(f)$ is an orthogonal increment process (Priestley, 1981, see also appendix B). The integral in (5) is a stochastic integral and hence only defined in the mean-square sense (see e.g. Priestley, 1981, ch. 3). We are particularly interested in the second moment of the process,

$$\mathrm{E}\{|\mathrm{d}Z(f)|^2\} = S(f)\mathrm{d}f, \tag{6}$$

which defines its spectral density function, $S(f)$. In addition, $\mathrm{d}Z$ is uncorrelated at different frequencies and

$$\mathrm{E}\{\mathrm{d}Z(f)\mathrm{d}Z^*(g)\} = S(f)\delta(f-g)\mathrm{d}f\mathrm{d}g. \tag{7}$$

Here, E denotes the expectation operator, * denotes complex conjugation and δ is the Dirac delta function. So far we have limited the discussion to zero-mean processes, i.e. $\mathrm{E}\{\mathrm{d}Z(f)\} = 0$, free of any periodic components. For many problems, harmonic oscillations are present in the time series being studied, and the underlying process is better described by the extended, or Munk-Hasselman (Munk & Hasselman, 1964), representation where the deterministic component of the process (i.e. its first moment) is given explicitly by

$$\mathrm{E}\{\mathrm{d}Z(f)\} = \sum_j \mu_j \delta(f-f_j)\mathrm{d}f, \tag{8}$$

where the f_j's are the frequencies of the periodic components and μ_j their amplitudes. The continuous, or background, part of the spectrum is given by the second central moment of $\mathrm{d}Z(f)$

$$S_c(f)\mathrm{d}f = \mathrm{E}\{|\mathrm{d}Z(f) - \mathrm{E}\{\mathrm{d}Z(f)\}|^2\}, \tag{9}$$

and describes the non-deterministic component of the process. Processes of this kind are known as centered or conditionally stationary and are said to have mixed spectra.

The distinction between the properties of first and second central moments is very important. First moments correspond to what is termed harmonic analysis, i.e. the study of periodic components. Typically, a process will contain a few such components, which can be described by their amplitude, frequency and phase (sometimes a frequency drift rate is also included). These parameters can be estimated using standard maximum-likelihood methods. The accuracy one can obtain in estimating frequencies of line components is a function of the local signal to noise ratio, defined as the ratio of power in the first moment to power in the second moment at each frequency. This means that in some cases it is possible to achieve resolution of the order of the Rayleigh resolution, $1/N$, for the line spectrum (and even do better than that) while typically the useful resolution for the continuum is between $2/N$ and $50/N$. When estimating the continuous spectrum, one is estimating a function of frequency. Its properties

set more stringent limits on the resolution that can be obtained (see Thomson, 1990a, and Thomson, 1990b, for details).

To study the statistical properties of the process $\mathrm{d}Z(f)$ we start by taking the discrete Fourier transform of the available data

$$\tilde{x}(f) = \sum_{t=0}^{N-1} x(t) \exp(-i2\pi ft), \tag{10}$$

and combine this with the spectral representation (5) to obtain

$$\tilde{x}(f) = \int_{-1/2}^{1/2} K_N(f-\nu)\mathrm{d}Z(\nu), \tag{11}$$

where the kernel (Dirichlet-kernel) is given by

$$K_N(f) = \sum_{t=0}^{N-1} \exp(-i2\pi ft) = \exp\left[-i2\pi f\frac{N-1}{2}\right]\frac{\sin N\pi f}{\sin \pi f}. \tag{12}$$

Equation (11) represents the fundamental equation of spectrum estimation and can be treated as a Fredholm integral equation of the first kind. Although it does not have a unique solution, approximate solutions will be constructed in section 4 and used to estimate the spectral density function. Note that $\tilde{x}(f)$ is a sufficient statistic since (10) may be inverse transformed to recover the data. This is however not the case for $|\tilde{x}(f)|^2$, i.e. the phase information, although not often quoted, is essential when reconstructing the time series, e.g. when removing harmonic components (see section 5).

The fundamental idea of the MTM is to obtain a set of uncorrelated spectrum estimates from a single time series by multiplying it in turn by each member of a set of orthogonal data tapers. The tapered series is then Fourier transformed, and finally the spectrum estimates so obtained are combined into a single one. The orthogonality of the windows, which are the Fourier transforms of the tapers, ensures that the spectrum estimates are uncorrelated under the assumption that the spectrum is constant over the bandwidth of the windows. This bandwidth is the only *ad hoc* parameter in the MTM, but methods for detecting unresolved structure are currently being developed to help choosing the appropriate bandwidth in each case (Thomson, 1990b).

4 Spectrum estimation as an inverse problem

It should be kept in mind, that in spectrum estimation one is interested in the statistical properties of the process, $\mathrm{d}Z(f)$, generating the time series, $x(t)$. Since the fundamental equation (11) is the frequency domain expression for the projection of an infinite stationary sequence generated by $\mathrm{d}Z(f)$ onto the finite sample, it does not have an inverse; hence, it is impossible to obtain exact or unique

solutions. As a result we must proceed by constructing approximate solutions which have statistical properties that, in some sense, resemble those of $\mathrm{d}Z(f)$, rather than resorting to studies of the statistical properties of the finite sample $\{x(t)\}_{t=0}^{N-1}$.

4.1 The Slepian functions

The key to the construction of such approximate solutions are the Slepian or discrete prolate spheroidal wave functions, whose properties are described by Slepian (1978) and Thomson (1990b, appendices A & B). These functions are the Fourier transforms of the so called discrete prolate spheroidal sequences (DPSS), or Slepian sequences, and it is instructive to see how one can construct those.

It is well known that multiplying a time series with a suitable taper before Fourier transforming gives superior results to those obtained by applying the Fourier transform directly. The primary purpose of data tapering is to reduce spectral leakage, i.e. minimize the energy contribution to a spectral component at frequency f from distant frequencies. The finite size of the sample at hand naturally sets some limits on the distance between mutually uncontaminated spectral components and thus controls the bandwidth ($2W$) of the window, or filter.

Consider a harmonic signal with angular frequency $\hat{\omega}$ and amplitude μ, $x(t) = \mu e^{i\hat{\omega}t}$. (Park *et al.*, 1987, and Lindberg & Park, 1987, consider a decaying signal, $x(t) = \mu e^{(i\hat{\omega}t-\alpha t)}$, the discussion below parallels theirs where we have set $\alpha = 0$.) A taper, $v(t)$, that maximizes the energy content of the tapered signal, $\{x(t)v(t)\}_{t=0}^{N-1}$, inside the interval $(\hat{\omega}-\Omega, \hat{\omega}+\Omega)$ where $\Omega = 2\pi W$, relative to the total energy must maximize the functional

$$\mathcal{F} = \frac{\int_{\hat{\omega}-\Omega}^{\hat{\omega}+\Omega} |x(\omega)|^2 \mathrm{d}\omega}{\int_{-\pi}^{\pi} |x(\omega)|^2 \mathrm{d}\omega}, \tag{13}$$

where $x(\omega)$ is the discrete Fourier transform of $\{x(t)v(t)\}_{t=0}^{N-1}$:

$$x(\omega) = \mu \sum_{t=0}^{N-1} \exp(-i\omega t) \exp(i\hat{\omega}t) v(t). \tag{14}$$

Since the time series is limited to $[0, N-1]$ it is impossible to confine the energy of its Fourier transform completely in $(\hat{\omega}-\Omega, \hat{\omega}+\Omega)$ and hence $\mathcal{F}$ will always be less than unity.

Expanding the numerator of (13) gives

$$\int_{\hat{\omega}-\Omega}^{\hat{\omega}+\Omega} |x(\omega)|^2 \mathrm{d}\omega \;=\; |\mu|^2 \int_{-\Omega}^{\Omega} \mathrm{d}\omega \sum_{t=0}^{N-1} \exp(-i\omega t) v(t) \times \sum_{s=0}^{N-1} \exp(-i\omega s) v(s)$$

$$= \quad 2|\mu|^2 \sum_{t=0}^{N-1} \sum_{s=0}^{N-1} v(t) \frac{\sin \Omega(s-t)}{(s-t)} v(s) \tag{15}$$

and by Parseval's theorem the denominator is

$$\int_{-\pi}^{\pi} |x(\omega)|^2 \mathrm{d}\omega = 2\pi |\mu|^2 \sum_{t=0}^{N-1} v^2(t). \tag{16}$$

Define the vector $\mathbf{v} = (v(0), v(1), \ldots, v(N-1))$, and the matrix $\mathbf{A}$ with elements

$$A_{lm} = \frac{\sin \Omega(l-m)}{\pi(l-m)}; \quad l, m = 0, 1, \ldots, N-1. \tag{17}$$

(Note that $\mathbf{A}$ is a symmetric Toeplitz matrix and thus has only N distinct elements.) Equation (13) can now be written in the compact form

$$\mathcal{F}(\mathbf{v}) = \frac{\mathbf{v}^{\mathrm{T}} \cdot \mathbf{A} \cdot \mathbf{v}}{\mathbf{v}^{\mathrm{T}} \cdot \mathbf{v}}, \tag{18}$$

where $^{\mathrm{T}}$ denotes transpose. To find the taper that maximizes the functional $\mathcal{F}$ set the variation of $\mathcal{F}$ with respect to $\mathbf{v}$ equal to zero

$$\delta \mathcal{F}(\mathbf{v}; \mathbf{h}) = \frac{\mathrm{d}}{\mathrm{d}\epsilon} \mathcal{F}(\mathbf{v} + \epsilon \mathbf{h}) \bigg|_{\epsilon=0} = 0 \tag{19}$$

for all N-vectors $\mathbf{h}$. This leads to the eigenvalue problem

$$\mathbf{A} \cdot \mathbf{v} = \lambda \mathbf{v}. \tag{20}$$

This equation has N eigenvalues and the corresponding eigenvectors are the discrete prolate spheroidal sequences which we set out to find. The DPSS are ordered by their eigenvalues, $1 > \lambda_0, \lambda_1, \ldots, \lambda_{N-1}$. The first $K = \lfloor 2NW \rfloor$ ($\lfloor \cdot \rfloor$ denoting the least integer or floor function) eigenvalues are exponentially close to 1. Hence, only the corresponding Slepian sequences can be used as data tapers since their spectral leakage, which is proportional to $1 - \lambda_k$, increases rapidly after that. Figure 1 shows the first 5 data tapers for a time-bandwidth product of 4 and the corresponding windows (Fourier transforms) are shown in figure 2. The tapers are designed for a 100 point series and hence the bandwidth of the windows is $2W = 8/100$ and a sharp cut-off is seen at $f = W = 4/100$.

There is a simpler and numerically more stable way to compute the Slepian sequences, first described by Slepian (1978) (see also Durrani & Chapman 1984; Thomson, 1990b). It is based upon a trigonometric series expansion of the solution to the differential equation for the discrete spheroidal wave functions. Using this expansion, the differential equation can be written as a second order difference equation for the successive terms in the series. In matrix form, this equation becomes

$$\boldsymbol{\sigma} \cdot \mathbf{v} = \theta \mathbf{v} \tag{21}$$

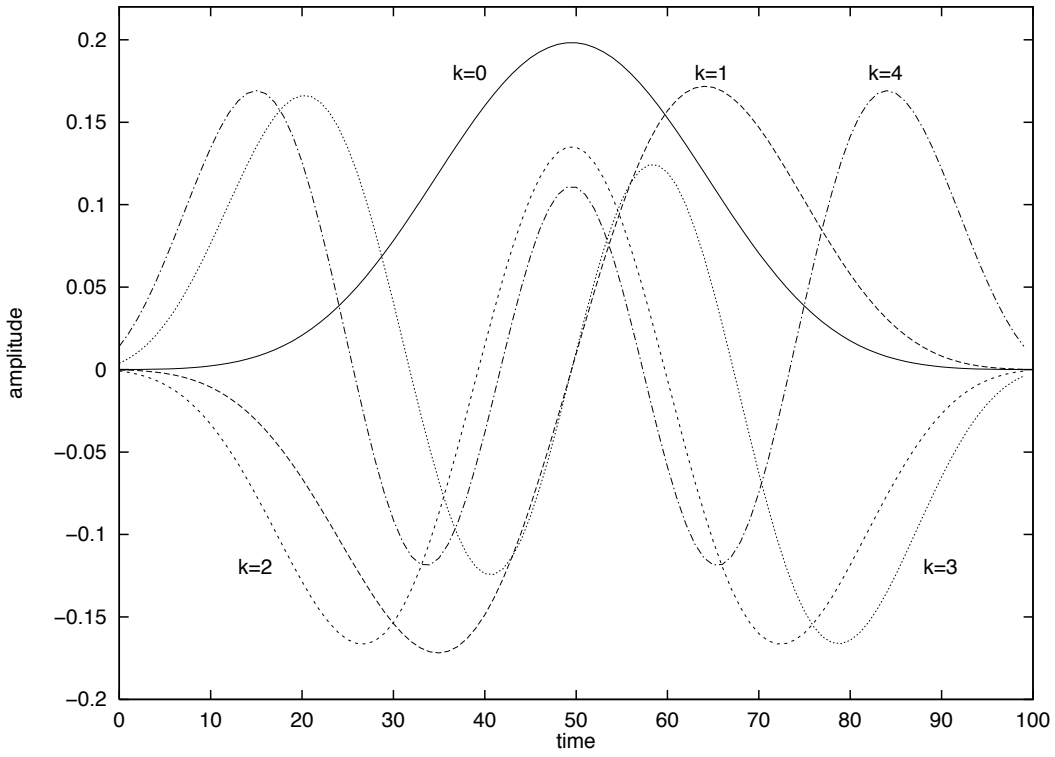

Figure 1: Discrete prolate spheroidal tapers for $N = 100, W = 0.04$.

where the matrix $\boldsymbol{\sigma}$ is tridiagonal and doubly symmetric with diagonal elements

$$\sigma_{ii} = (\tfrac{1}{2}(N-1) - i)^2 \cos(2\pi W) \quad i = 0, \ldots, N-1 \tag{22}$$

and off-diagonal elements

$$\sigma_{i,i-1} = \sigma_{i-1,i} = \tfrac{1}{2} i(N-i) \quad i = 1, \ldots, N-1. \tag{23}$$

One proceeds by finding the eigenvalues, $\{\theta\}_{i=1}^{N}$, of $\boldsymbol{\sigma}$, using a standard routine for tridiagonal matrices (e.g. *tqli* from Press *et al.*, 1988) and then finding the Slepian sequences by recursively solving

$$(\boldsymbol{\sigma} - \theta_k \mathbf{I}) \cdot \mathbf{v}_k = 0 \tag{24}$$

for each of the K highest eigenvalues of $\boldsymbol{\sigma}$. Here $\mathbf{I}$ is the $N \times N$ identity matrix. We start by choosing $v_k(0) = 1$ and set $v_k(-1) = 0$. The series are then normalized to have $\mathbf{v}_k^{\mathrm{T}} \cdot \mathbf{v}_k = 1$ and the sign chosen such that even series are positive at the center of the range and odd sequences have positive central slope. The exact sign convention varies somewhat in the literature (compare e.g. Fig. 1 in Thomson, 1982, and Figure 1 in Park *et al.*, 1987) but here we follow Thomson (1990b).

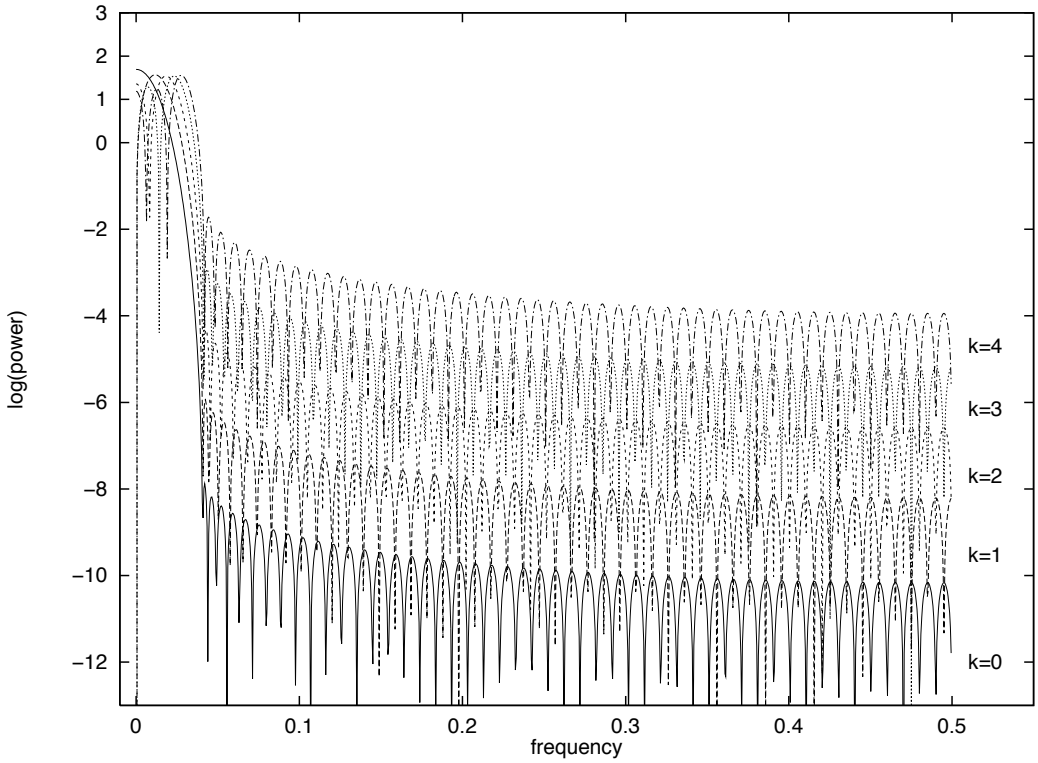

Figure 2: Prolate windows corresponding to the tapers in figure 1.

Thomson (1990b) gives a formula for evaluating the eigenvalues corresponding to the Slepian functions,

$$\lambda_k = \frac{\int_{-W}^{W} |V_k(f)|^2 \mathrm{d}f}{\int_{-1/2}^{1/2} |V_k(f)|^2 \mathrm{d}f} \tag{25}$$

where the Slepian functions, $V_k(f)$, are the Fourier transforms of the Slepian sequences, $\{v_k(t)\}_{k=0}^{N-1}$,

$$V_k(f) = \sum_{t=0}^{N-1} v_k(t) \exp(-i2\pi ft). \tag{26}$$

They are also solutions of the integral equation

$$\lambda_k V_k(f) = \int_{-W}^{W} K_N(f-\nu) V_k(\nu) \mathrm{d}\nu, \tag{27}$$

where the kernel is again given by (12). Note that the phase of the functions $V_k(f)$ is different from the original Slepian functions, $U_k(f)$, which are used in

Thomson (1982),

$$V_k(f) = \frac{1}{\epsilon_k} \exp\left[-i2\pi f \frac{N-1}{2}\right] U_k(-f), \tag{28}$$

where $\epsilon_k = 1$ for k even and $\epsilon_k = i$ for k odd. This is done to agree with common definitions of the discrete Fourier transform. Also, to be precise, one would need to make the dependence of the v_k's (and λ_k's, V_k's etc.) on N and W clear by writing $v_k(t; N, W)$ etc. This notation will be suppressed here for simplicity and the reader asked to bear this dependence in mind.

The functions $\{V_k(f)\}_{k=0}^{N-1}$, which are the eigenfunctions of $K_N(f-\nu)$, are doubly orthogonal, i.e. they are orthogonal over $(-W, W)$,

$$\int_{-W}^{W} V_j(f) V_k^*(f) \mathrm{d}f = \lambda_k \delta_{kj}, \tag{29}$$

and orthonormal over the entire frequency range $(-\frac{1}{2}, \frac{1}{2})$,

$$\int_{-1/2}^{1/2} V_j(f) V_k^*(f) \mathrm{d}f = \delta_{kj}. \tag{30}$$

When combined, these two orthogonality properties give the eigenvalue formula (25). Also note that similar orthogonality relations hold for the DPSS, i.e. they are orthogonal on $(-\infty, \infty)$ and orthonormal on $[0, N-1]$ (Thomson, 1982). The DPSS are optimal tapers in the sense that of all sets of K orthonormal sequences of duration N, their Fourier transforms (i.e. the Slepian functions) have the maximum energy concentration in the bandwidth $(-W, W)$.

4.2 Construction of the spectrum estimate

The Slepian functions introduced above form a complete set in the class of bandlimited functions, i.e. functions with finite power and whose spectrum vanishes outside some finite interval $(-\sigma, \sigma)$ (Papoulis, 1984). This means that all bandlimited functions can be expanded in the Slepian basis functions. Hence, the observable portion of $\mathrm{d}Z$ can be assumed to have the expansion

$$\mathrm{d}Z(f-\nu) = \sum_{k=0}^{\infty} X_k(f) V_k^*(\nu) \mathrm{d}\nu, \tag{31}$$

for $|\nu| < W$ (Thomson 1990a). By the assumed stationarity, the part of $\mathrm{d}Z$ in the local domain, $(f-W, f+W)$, is uncorrelated with $\mathrm{d}Z$ in the rest of the frequency domain. Multiplying (31) with $V_j(\nu)$ and integrating over $(-W, W)$ gives

$$X_k(f) = \frac{1}{\sqrt{\lambda_k}} \int_{-W}^{W} V_k(\nu) \mathrm{d}Z(f-\nu) \tag{32}$$

where we have used the orthogonality property, equation (29), and normalized the coefficients, $X_k(f)$, in such a way that $\mathrm{E}\{|X_k(f)|^2\} = \sigma^2$ if the spectrum $S(f)$ is white with variance σ^2. Although unobservable, the $X_k(f)$'s are of considerable analytic interest since they are the expansion coefficients that would be obtained if the entire time series were passed through an ideal bandpass filter, from $f-W$ to $f+W$, before truncating it to the finite sample (Thomson, 1982).

Using the above assumption, (31), together with the fundamental equation, (11), and the orthonormality property of the tapers, $v_k(t)$, the expansion or eigencoefficients for the finite time series can be calculated:

$$\begin{aligned} x_k(f) &= \int_{-1/2}^{1/2} V_k(\nu)\mathrm{d}Z(f-\nu) \\ &= \sum_{t=0}^{N-1} \exp(-i2\pi ft)v_k(t)x(t), \end{aligned} \tag{33}$$

giving an estimate of the coefficients $X_k(f)$. We shall see later how one can minimize the mean square error between $X_k(f)$ and $x_k(f)$. In addition to the change in integration interval, a factor of $1/\sqrt{\lambda_k}$ is included in (32) to preserve the orthonormality on the inner interval $(-W, W)$ (details are in Thomson, 1990b).

Note that the estimated expansion coefficients, $x_k(f)$, are obtained by Fourier transforming the tapered time series. In pratice, the tapered series is zero padded to length $N_{\mathrm{FFT}} = 2^m$, i.e. $x(t)$ is set to 0 for $t = N, \ldots, N_{\mathrm{FFT}} - 1$. The number m depends on the interpolation wanted, typically $2N \leq N_{\mathrm{FFT}} \leq 10N$. The Fourier transforms are then calculated on a mesh from $f = 0$ to $f = 1/2$ (Nyquist frequency) with $\Delta f = 1/2N_{\mathrm{FFT}}$ using a standard FFT routine (e.g. *realft* from Press *et al.*, 1988). The absolute squares of the expansion coefficients,

$$\hat{S}_k(f) = |x_k(f)|^2, \tag{34}$$

are individually direct spectrum estimates and the set $\{\hat{S}_k(f)\}_{k=0}^{K-1}$ can be used to estimate the statistical properties of the spectrum which is formed by combining this set of eigenspectra into a single conglomeration.

As mentioned earlier, only the first $K = \lfloor 2NW \rfloor$ Slepian functions have low spectral leakage and hence only those (or fewer) are used when constructing the spectrum estimate. Of all functions which are the Fourier transform of an index limited sequence, the function $V_0(f)$ has the greatest fractional energy concentration in $(-W, W)$ and hence using only that function is comparable to standard filtering techniques where one filter is used. However, by combining the first K expansion coefficients corresponding to the highest eigenvalues, one obtains a spectrum estimate with typically $2K$ degrees of freedom instead of 2 when using conventional methods. To see how this is possible consider a crude multiple-window spectrum estimate given by the average of the first K eigenspectra,

$$\bar{S}(f) = \frac{1}{K}\sum_{k=0}^{K-1} \hat{S}_k(f), \tag{35}$$

and temporarily restrict the discussion to the continuous part of the spectrum. The second moment, or covariance, of the eigencoefficients is given by

$$\begin{aligned} \mathrm{E}\{x_j(f)x_k^*(f')\} &= \mathrm{E}\left\{\int_{-1/2}^{1/2}\int_{-1/2}^{1/2} V_j(\zeta)V_k^*(\xi)\mathrm{d}Z(f-\zeta)\mathrm{d}Z^*(f'-\xi)\right\} \\ &= \int_{-1/2}^{1/2} V_j(f-\zeta)S(\zeta)V_k^*(f'-\zeta)\mathrm{d}\zeta. \end{aligned} \tag{36}$$

where we have used (7) to perform the integration. From this and the orthogonality of the prolate functions it is clear that if the spectrum, $S(f)$, is reasonably flat within $(f-W, f+W)$ the eigencoefficients at each frequency are uncorrelated,

$$\mathrm{E}\{x_j(f)x_k^*(f)\} \approx S(f)\delta_{jk}. \tag{37}$$

Considerable correlation can however arise if the spectrum is highly variable in this region. Assuming a locally flat spectrum and a Gaussian process $\mathrm{d}Z(f)$, the estimate (35) is a sum of K squares of Gaussian variables at each frequency. Hence, each term in the sum is distributed as chi-square with 2 degrees of freedom, ξ_2^2, and contributes 2 degrees of freedom to the spectrum estimate.

The use of the first $K \leq \lfloor 2NW \rfloor$ windowed estimates thus results in a spectrum estimate with $2K$ degrees of freedom, without reducing the resolution, W. This is in contrast with earlier methods where convolution smoothers have been essential to give consistent spectrum estimates, with the cost of poorer resolution. Typically W is chosen between $1/N$ and $25/N$ with a time-bandwidth product, NW, of 4 or 5 being a common starting point. With $W = 4/N$ or $5/N$, K is usually taken conservatively as 6 or 8, giving estimates with 12 or 16 degrees of freedom respectively. This range of W is chosen in accordance with the achievable resolution for the continuum (cf. the discussion in section 3).

In practice, a more complicated combination of the eigenspectra than the arithmetic mean (35) is used. Thomson (1982, §V) describes a data adaptive weighting scheme which gives an optimal solution in the sense that it minimizes the mean square error between the estimated eigencoefficients, $x_k(f)$, and the "exact" ones, $X_k(f)$. Qualitatively, it can be envisaged that since the spectral leakage of the prolate filters $V_k(f)$ increases with k, and the bias characteristics of the corresponding eigenspectra degrade, the higher order eigenspectra will have to be downweighted relative to the lower order ones, especially in regions where the spectrum is low. This is done by introducing a sequence of weight functions, $d_k(f)$, that modify the corresponding eigencoefficients. We thus consider the difference

$$\begin{aligned} X_k(f) - d_k(f)x_k(f) &= \frac{1}{\sqrt{\lambda_k}}\int_{-W}^{W} V_k(\zeta)\mathrm{d}Z(f-\zeta) - d_k(f)\int_{-1/2}^{1/2} V_k(\zeta)\mathrm{d}Z(f-\zeta) \\ &= \left(\frac{1}{\sqrt{\lambda_k}} - d_k(f)\right)\int_{-W}^{W} V_k(\zeta)\mathrm{d}Z(f-\zeta) \\ &\quad - d_k(f)\oint\!\!\!\!\!\!\int V_k(\zeta)\mathrm{d}Z(f-\zeta) \end{aligned} \tag{38}$$

where we have collected regions of integration and the cut-integral is defined by

$$\not\int = \int_{-1/2}^{1/2} - \int_{-W}^{W}. \tag{39}$$

The error consists of two terms which both are integrals with respect to the random process $\mathrm{d}Z$ but the first one is over $(-W, W)$ while the latter is an integral over the remainder of the principal domain. This means that the two terms are independent and their mean square error is hence the sum of their squares. Assuming that the spectrum, $S(f)$, varies slowly over the local domain, the square of the first term is well approximated by

$$\mathrm{E}\left\{\left|\int_{-W}^{W} V_k(\zeta)\mathrm{d}Z(f-\zeta)\right|^2\right\} \approx \lambda_k S(f). \tag{40}$$

The square of the second integral in (38) is termed broad band bias by Thomson (1982) and denoted by $B_k(f)$. The integral of its average value over all frequencies is given by

$$\int_{-1/2}^{1/2} \mathrm{E}\{B_k(f)\}\mathrm{d}f = \sigma^2(1-\lambda_k) \tag{41}$$

where σ^2 is the process variance

$$\sigma^2 = \int_{-1/2}^{1/2} S(f)\mathrm{d}f. \tag{42}$$

In the mtm-program described in appendix A, an initial estimate of the variance, $\hat{\sigma}^2$, is obtained from the variance of the data. After line components have been removed (see section 5), the variance is estimated by integrating the background spectral density function with a discrete version of (42). It should be noted that the spectrum estimates considered here do not conserve power rigorously so that Parseval's theorem is only satisfied approximately in expected value (Thomson, 1990b).

Combining these two integrals and minimizing the mean square error with respect to $d_k(f)$ gives the approximate optimum weights

$$d_k(f) = \frac{\sqrt{\lambda_k}S(f)}{\lambda_k S(f) + \mathrm{E}\{B_k(f)\}}, \tag{43}$$

the corresponding average of the spectral density function being

$$\hat{S}(f) = \frac{\sum_{k=0}^{K-1} |d_k(f)|^2 \hat{S}_k(f)}{\sum_{k=0}^{K-1} |d_k(f)|^2}. \tag{44}$$

Since the (obviously unknown) values of the spectrum appear in the expression for the weight functions, both directly and implicitly through the dependence of the estimate of the broad band bias, we replace $S(f)$ with the estimate $\hat{S}(f)$. The formula for $d_k(f)$, (43), and equation (44) are then used recursively until convergence is achieved. The criterion used in the program to stop this iteration is that

$$\max_k \left| \frac{d_k^{(i)} - d_k^{(i+1)}}{d_k^{(i)}} \right| < 0.01. \tag{45}$$

The average of the first two eigenspectra is used as an initial estimate for $S(f)$ and the resulting spectrum estimate is a solution of the equation

$$\sum_{k=0}^{K-1} \frac{\lambda_k(\hat{S}(f) - \hat{S}_k(f))}{[\lambda_k \hat{S}(f) + \hat{B}_k(f)]^2} = 0 \tag{46}$$

where $\hat{B}_k(f)$ is an estimate of the broad band bias. Currently, this is approximated by its average value $\hat{\sigma}^2(1-\lambda_k)$ in the program. (Thomson (1982) gives some further comments on refinements.) The phase corresponding to the spectrum estimate $\hat{S}$ is obtained from the phase of the weighted coefficients,

$$\phi(f) = \frac{\sum_{k=0}^{K-1} d_k(f) x_k(f)}{\left| \sum_{k=0}^{K-1} d_k(f) x_k(f) \right|}. \tag{47}$$

In the program, the phase spectrum $\phi(f)$ of the continuum is calculated, and phases of significant harmonic components are also quoted (see section 5 and appendix A).

A useful by-product of the above estimation procedure is

$$v(f) = 2 \sum_{k=0}^{K-1} |d_k(f)|^2, \tag{48}$$

which gives the approximate degrees of freedom for the estimate $\hat{S}(f)$ as a function of frequency. This provides a way to select a proper bandwidth for the problem at hand since if the average of $v(f)$ is significantly less than $2K$ then either W is too small or additional prewhitening of the data is needed. The exact meaning of "significantly" is not quite clear and a more rigorous way of selecting the proper bandwidth is to test for unresolved structure in the local domain. Inferences about this can be obtained from quadratic inverse theory (Thomson, 1990b).

The jackknifing method, outlined in appendix B, is used to obtain confidence intervals on the spectrum estimate. This is done by jackknifing the logarithm of

the spectrum. First we calculate the delete-one values,

$$\log \hat{S}_{(j)} = \log \left(\sum_{\substack{k=0 \\ k \neq j}}^{K-1} |d_k(f)|^2 \hat{S}_k(f) \Big/ \sum_{\substack{k=0 \\ k \neq j}}^{K-1} |d_k(f)|^2 \right), \tag{49}$$

and form their average

$$\log \hat{S}_{(\cdot)} = \frac{1}{K} \sum_{j=1}^{K-1} \log \hat{S}_{(j)}. \tag{50}$$

The jackknife estimate of the variance of $\log \hat{S}$ is then

$$\begin{aligned} \tilde{\sigma}^2 &= \mathrm{var}(\log \hat{S}) \\ &= \frac{K-1}{K} \sum_{i=0}^{K-1} \left(\log \hat{S}_{(i)} - \log \hat{S}_{(\cdot)} \right)^2 \end{aligned} \tag{51}$$

and because of the logarithmic transformation, the ratio $(\log \hat{S}_{(i)} - \log \hat{S}_{(\cdot)})/\tilde{\sigma}$ is nearly distributed as t_{K-1}, where t denotes Student's t-distribution. Hence, the double-sided $1-\alpha$ confidence interval for the power spectrum is (Thomson & Chave, 1990)

$$\hat{S} \exp\left(-t_{K-1} \left(1 - \frac{\alpha}{2} \right) \tilde{\sigma} \right) \leq S \leq \hat{S} \exp\left(t_{K-1} \left(1 - \frac{\alpha}{2} \right) \tilde{\sigma} \right). \tag{52}$$

The jackknife bias estimate on $\log \hat{S}$ is also calculated in the program. According to Thomson (1990b) it is given by

$$\log \hat{B} = (K-1)(\log \hat{S}_{(\cdot)} - \log \hat{S}). \tag{53}$$

This bias estimate can be compared with theoretical calculations based on Gaussian assumptions (see appendix A). Note that in the last few formulas the frequency dependence has been dropped for clarity.

In this section, the main emphasis has been on estimating the continuous spectrum or the spectral density function, $S_c(f)$. As mentioned in section 3, the first moment of the process describes its deterministic part and hence is of great importance if harmonic oscillations are present in the data.

5 Harmonic analysis

It is quite common in spectral analysis to have spectra consisting of sharp line components embedded in continuous spectra. The lines can be due to some periodic forcing, as is the case with the the annual variation of ozone, or be an intrinsic property of the system as in the case of dHvA oscillations in the properties of the Fermi surfaces of metals. To model such mixed spectra we assume

that the process has a non-zero mean value function consisting of a number of sinusoids at various frequencies (see equation (8)). The MTM allowes one to estimate the amplitude of the line components and provides an analysis-of-variance test for their significance.

Evaluating (33) gives

$$\begin{aligned} \mathrm{E}\{x_k(f)\} &= \sum_{t=0}^{N-1} \exp(-i2\pi ft) v_k(t) \mathrm{E}\{x(t)\} \\ &= \sum_{t=0}^{N-1} \exp(-i2\pi ft) v_k(t) \sum_j \mu_j \exp(i2\pi f_j t) \\ &= \sum_j \mu_j V_k(f - f_j) \end{aligned} \tag{54}$$

where we have used equations (5), (8) and (26). We found earlier that if the continuous spectrum, $S_c(f)$, does not vary too rapidly over $(f - W, f + W)$, the different eigencoefficients were approximately uncorrelated (see equation (37)). Thus if the line frequencies were known, one could find the amplitudes by minimizing

$$\sum_{f,k} |x_k(f) - \sum_j \mu_j V_k(f - f_j)|^2. \tag{55}$$

If the different line frequencies are separated by at least W, this minimization results in a matrix which is strongly diagonal by virtue of the orthogonality of the Slepian functions and their energy concentration. In this case the coefficients μ_j can be estimated independently of each other. Under this assumption it is therefore sufficient to consider the simple case of a single, isolated line at frequency f_0. Since $\mathrm{E}\{x_k(f_0)\} = \mu_0 V_k(0)$ one may estimate μ_0 given f_0 by ordinary least-squares. The presence of this line is then tested with a generalized likelihood ratio test,

$$\max \frac{L(\{X\}|\mu)}{L(\{X\}|\mu = 0)}, \tag{56}$$

that, under a Gaussian assumption, becomes the variance ratio test (Thomson, 1990b).

To estimate the amplitude of a single line at frequency f_0 we minimize the mean square error between the observed eigencoefficients and their expected values

$$M = \sum_{k=0}^{K-1} |x_k(f) - \hat{\mu}_0 V_k(f - f_0)|^2 \tag{57}$$

at f_0, i.e. solve $(\partial M / \partial \mu_0^*)|_{f=f_0} = 0$. This results in the simple linear regression

estimate

$$\hat{\mu}_0 = \frac{\sum_{k=0}^{K-1} V_k^*(0) x_k(f_0)}{\sum_{k=0}^{K-1} |V_k(0)|^2}. \tag{58}$$

The significance of this estimate may be tested by using a standard F-test. Taking the ratio of the variance explained by the line to the unexplained variance, normalized by their respective degrees of freedom, one obtains

$$F(f) = \frac{(2K-\nu)|\hat{\mu}(f)|^2 \sum_{k=0}^{K-1} |V_k(0)|^2}{\nu \sum_{k=0}^{K-1} |x_k(f) - \hat{\mu}(f) V_k(0)|^2} \tag{59}$$

where the constant factors $(2K-\nu)$ and ν provide proper scaling for F with ν and $2K-\nu$ degrees of freedom. For testing at a known frequency $\nu = 2$ but if the frequency is estimated as well $\nu = 3$ (Thomson, 1990b).

From the symmetry of the Slepian sequences it is clear that $V_k(0) = 0$ for k odd, indicating that in (58) only even terms contribute to $\hat{\mu}_0$. The integral regression method proposed in Thomson (1982) overcomes this drawback by minimizing the integral of the error, M, over the band $(f_0 - W, f_0 + W)$. Both estimates and a range of intermediate forms can be covered by including a weight function, w, in the integral for the integrated error (Lindberg & Park, 1987; Thomson, 1990b)

$$M_I = \int_{\hat{f}-W}^{\hat{f}+W} \sum_{k=0}^{K-1} |x_k(f) - \hat{\mu}_I V_k(f - \hat{f})|^2 w(f - \hat{f}) \mathrm{d}f. \tag{60}$$

The point estimate then corresponds to $w(f) = \delta(f)$ and the integrated form to $w(f) = 1$. Obviously, this integration increases the bandwidth of the estimate from $\hat{f} \pm W$ to $\hat{f} \pm 2W$ (since the $x_k(f)$'s are smeared over $f \pm W$, see also Fig. 20 in Thomson, 1982). However, the effective sidelobes of the integrated estimate are very low.

With the weighted integration the above formulas for $\hat{\mu}_0$ and F become

$$\hat{\mu}_I(\hat{f}) = \frac{\sum_{k=0}^{K-1} \int_{\hat{f}-W}^{\hat{f}+W} V_k^*(f - \hat{f}) x_k(f) w(f - \hat{f}) \mathrm{d}f}{\sum_{k=0}^{K-1} \int_{\hat{f}-W}^{\hat{f}+W} |V_k(f - \hat{f})|^2 w(f - \hat{f}) \mathrm{d}f} \tag{61}$$

and

$$F_I(\hat{f}) = \frac{(2K-\nu)|\hat{\mu}_I(\hat{f})|^2 \sum_{k=0}^{K-1} \int_{\hat{f}-W}^{\hat{f}+W} |V_k(f - \hat{f})|^2 w(f - \hat{f}) \mathrm{d}f}{\nu \sum_{k=0}^{K-1} \int_{\hat{f}-W}^{\hat{f}+W} |x_k(f) - \hat{\mu}_I V_k(f - \hat{f})|^2 w(f - \hat{f}) \mathrm{d}f}. \tag{62}$$

The F's and $\hat{\mu}$'s are then evaluated at the FFT bin frequencies, $\{f_n\}_{n=0}^{N_{\rm FFT}-1}$.

In the mtm-program, only the unweighted integral and point regression forms are used, i.e. $w(f) = 1$ and $w(f) = \delta(f)$. For the integral form we have from (29) that

$$\sum_{k=0}^{K-1} \int_{\hat{f}-W}^{\hat{f}+W} |V_k(f-\hat{f})|^2 \mathrm{d}f = \sum_{k=0}^{K-1} \lambda_k. \tag{63}$$

Also, it is easy to show that

$$\sum_{k=0}^{K-1} \int_{\hat{f}-W}^{\hat{f}+W} V_k^*(f-\hat{f}) x_k(f) \mathrm{d}f = \sum_{k=0}^{K-1} \lambda_k \sum_{t=0}^{N-1} x(t) v_k^2(t) \exp(-i2\pi f t) \tag{64}$$

and hence this term can be calculated efficiently using FFT. The only term which is not easily evaluated is

$$\begin{aligned} \sum_{k=0}^{K-1} \int_{\hat{f}-W}^{\hat{f}+W} |x_k(f)|^2 \mathrm{d}f &= 2 \sum_{k=0}^{K-1} \sum_{t=0}^{N-1} \sum_{s=0}^{N-1} x(t) x(s) v_k(t) v_k(s) \\ &\quad \times \exp(i2\pi \hat{f}(t-s)) \times \frac{\sin 2\pi W(t-s)}{(t-s)}. \end{aligned} \tag{65}$$

In fact the denominator in (62) is evaluated with numerical integration in the program, since negative values can occur if the absolute value is expanded and the above formulas used to simplify the results (see Appendix A for details).

The jackknife method is applied to the point regression F-test values to estimate the variance of the estimated line frequencies. We start by forming the delete-one F-test values, given by

$$F_{(j)}(f) = \frac{(2K-\nu)|\hat{\mu}(f)|^2 \sum_{\substack{k=0 \\ k \neq j}}^{K-1} |V_k(0)|^2}{\nu \sum_{\substack{k=0 \\ k \neq j}}^{K-1} |x_k(f) - \hat{\mu}(f) V_k(0)|^2}. \tag{66}$$

Denote by $f_{(j)}^{\rm line}$ the frequency of a maximum in $F_{(j)}(f)$, that reaches the F-test criterion imposed. The jackknife mean and variance of such a frequency is then given by

$$f_{(\cdot)}^{\rm line} = \frac{1}{K} \sum_{j=0}^{K-1} f_{(j)}^{\rm line} \tag{67}$$

and

$$\mathrm{var}\{f_{(j)}^{\rm line}\} = \frac{K-1}{K} \sum_{j=0}^{K-1} \left(f_{(j)}^{\rm line} - f_{(\cdot)}^{\rm line} \right)^2, \tag{68}$$

respectively. (These values are quoted in columns 2 and 3 in the *.info* file as described in appendix A.)

The significance level of the F-test can be calculated using

$$P(F|\nu_1,\nu_2) = 1 - I_{\frac{\nu_2}{\nu_2+\nu_1 F}}(\nu_2/2,\nu_1/2) \tag{69}$$

where in our case $\nu_1 = \nu$ and $\nu_2 = 2K - \nu$. Here, $I_x(a,b)$ is the incomplete beta function (for details, see Press *et al.*, ch. 6). The significance level at which the hypothesis "variance of line component is smaller than unexplained variance" can be rejected is $1 - P$, with a low numerical value implying a very significant rejection. Thus, P-values close to 1 imply a highly significant line component.

Thomson (1990b) gives some very good comments on the F-test in §5 of his paper and some of these are restated below. Thomson points out that one should pad the time series to $4 - -10N$ since strong periodic signals could be missed if a coarser mesh were used. The frequency estimate of the lines, deduced from maxima of the F-test, can be refined further by using a single frequency Fourier transform (this is not implemented in the program yet). Secondly, one should be cautious in declaring significant lines since random fluctuations can also give rise to high F-test values. A rule of thumb is to use $1 - 1/N$ as a lower bound on the significance level (Thomson, 1990a). The single-line F-test will usually fail on multiple lines when they are spaced less than W apart. Thomson (1990b, §6) describes a multiple line F-test, which will be implemented in the program in the future. Finally, it is convenient to reshape the spectral density by removing the effects of the significant harmonic components and insert the corresponding lines into the spectrum. This is done by replacing the $x_k(f)$'s with $x_k(f) - \hat{\mu}_j V_k(f - f_j)$ for each of the lines and forming the background spectrum as explained in section 4. Each line is then superposed by adding a portion with the shape of the corresponding F line (out to the next local minimum) scaled in to preserve power. The width of the line is thus proportional to the frequency uncertainty of the estimate.

6 Cross-spectral analysis

When analysing a complex physical system, e.g. the atmosphere, we are not only interested in the spectral properties of each variable that characterizes the system but also in the interrelationships between these variables. To describe the relation between two random processes, an analogous concept to the joint probabilty distribution for random variables is needed. This is achieved by introducing the cross-spectrum which represents the covariance between the two processes.

Consider two random processes $X_1(t)$ and $X_2(t)$ that satisfy

(i) $X_1(t)$ and $X_2(t)$ are stationary
(ii) $\mathrm{cov}\{X_1(t), X_2(s)\} = \mathrm{E}\{X_1(t)X_2^*(s)\}$ is a function of $(s-t)$ only.

Here, cov$\{\cdot\}$ denotes the covariance operator. The two processes are then said to be jointly stationary and below we shall only be dealing with such processes. Condition (ii) then tells us that the cross-covariance function

$$\begin{aligned} R_{12}(s) &= \mathrm{E}\{X_2^*(t)X_1(t+s)\} && (70)\\ &= \int_{-1/2}^{1/2}\int_{-1/2}^{1/2} e^{-i2\pi ft}e^{i2\pi f'(t+s)}\mathrm{E}\{\mathrm{d}Z_2^*(f)\mathrm{d}Z_1(f')\} && (71)\end{aligned}$$

is a function of s only. The right hand side must thus not depend on t and this can only be so if the contribution to the double integral is 0 when $f \neq f'$. The two processes are hence not only orthogonal but also cross-orthogonal, i.e.

$$\mathrm{E}\{\mathrm{d}Z_2^*(f)\mathrm{d}Z_1(f')\} = 0 \quad \text{if } f \neq f'. \tag{72}$$

Using this property (71) reduces to

$$R_{12}(s) = \int_{-1/2}^{1/2} e^{i2\pi fs}\mathrm{E}\{\mathrm{d}Z_2^*(f)\mathrm{d}Z_1(f)\}. \tag{73}$$

It is now convenient to introduce a special notation for ordinary spectra, or auto-spectra. We denote the spectra of the two processes by

$$S_{11}(f)\mathrm{d}f = \mathrm{E}\{|\mathrm{d}Z_1(f)|^2\}, \qquad S_{22}(f)\mathrm{d}f = \mathrm{E}\{|\mathrm{d}Z_2(f)|^2\} \tag{74}$$

and define their cross-spectral density by

$$S_{12}(f)\mathrm{d}f = \mathrm{E}\{\mathrm{d}Z_2^*(f)\mathrm{d}Z_1(f)\}. \tag{75}$$

The interpretation of this function is that it represents the average value of the product of the coefficients of $e^{i2\pi ft}$ in $X_1(t)$ and $X_2(t)$. Alternatively, we can say that whereas $S_{11}(f)\mathrm{d}f$, $S_{22}(f)\mathrm{d}f$ represent the variance of $\mathrm{d}Z_1(f)$, $\mathrm{d}Z_2(f)$ respectively, $S_{12}(f)\mathrm{d}f$ represents the covariance between $\mathrm{d}Z_1(f)$ and $\mathrm{d}Z_2(f)$ (Priestley, 1981).

To investigate further the interpretation of the cross-spectrum write it in polar form

$$S_{12}(f)\mathrm{d}f = \alpha_{12}(f)\exp(i2\pi\phi_{12}(f)) \tag{76}$$

and similarly

$$\mathrm{d}Z_i = |\mathrm{d}Z_i|\exp(i2\pi\phi_i(f)). \tag{77}$$

Combining these two equations gives

$$\alpha_{12}(f)\exp(i2\pi\phi_{12}(f)) = \mathrm{E}\{|\mathrm{d}Z_1||\mathrm{d}Z_2|\}\mathrm{E}\{\exp(i2\pi(\phi_1(f) - \phi_2(f)))\} \tag{78}$$

This relation defines explicitly the meaning of the average value interpretation stated above.

We now define the complex coherency (at frequency f) by

$$w_{12}(f) = \frac{S_{12}(f)}{\left(S_{11}(f)S_{22}(f)\right)^2}. \tag{79}$$

and coherence is then defined as $|w_{12}|$. Using the above definitions of the auto-spectra and cross-spectrum, (79) can be rewritten as

$$w_{12}(f) = \frac{\mathrm{cov}\{\mathrm{d}Z_1(f), \mathrm{d}Z_2(f)\}}{\left(\mathrm{var}\{\mathrm{d}Z_1(f)\}\mathrm{var}\{\mathrm{d}Z_2(f)\}\right)^{1/2}} \tag{80}$$

so that $w_{12}(f)$ may be interpreted as the correlation coefficient between the random coefficients of the components in $X_1(t)$ and $X_2(t)$ at frequency f. It follows immediately that for all f

$$0 \leq |w_{12}(f)| \leq 1 \tag{81}$$

for any two jointly stationary processes. As in the case of ordinary correlation coefficients the closeness of $|w_{12}(f)|$ to unity indicates the extent to which the random coefficients (at frequency f) are linearly related. The form of $|w_{12}(f)|$ over all frequencies determines the extent to which the processes $X_1(t)$ and $X_2(t)$ are linearly related (Priestley, 1981). The coherence can thus be thought of as a correlation coefficient in the frequency domain. It is easy to show that w_{12} is invariant under linear transformations of $X_1(t)$ and $X_2(t)$, just as in the case of two ordinary random variables.

The interpretation of the phase spectrum $\phi_{12}(f)$ is best illustrated with the following example. Consider two stationary random processes, $X_1(t)$ and $X_2(t)$, that satisfy a linear regression relationship but with time delay d,

$$X_1(t) = aX_2(t-d) + \epsilon(t), \tag{82}$$

where $\epsilon(t)$ is white noise, uncorrelated with $X_2(t)$. Using (5) gives

$$\begin{aligned} X_2(t-d) &= \int_{-1/2}^{1/2} e^{i2\pi f(t-d)}\mathrm{d}Z_2(f) && (83)\\ &= \int_{-1/2}^{1/2} e^{i2\pi ft}\left(e^{-i2\pi fd}\mathrm{d}Z_2(f)\right) && (84) \end{aligned}$$

so that

$$\mathrm{d}Z_1 = ae^{-i2\pi fd}\mathrm{d}Z_2 + \mathrm{d}Z_\epsilon. \tag{85}$$

Since $\mathrm{d}Z_2$ and $\mathrm{d}Z_\epsilon$ are uncorrelated the cross-spectrum can be expressed in terms of the auto-spectra, e.g.

$$\begin{aligned} S_{12}(f)\mathrm{d}f &= \mathrm{E}\{\mathrm{d}Z_2^*\mathrm{d}Z_1\} && (86)\\ &= ae^{-i2\pi fd}\mathrm{E}\{|\mathrm{d}Z_2|^2\} && (87)\\ &= ae^{-i2\pi fd}S_{22}(f)\mathrm{d}f. && (88) \end{aligned}$$

From this expression we can read off the amplitude and phase of $S_{12}(f)$,

$$\alpha_{12}(f) = aS_{22}(f), \qquad \phi_{12}(f) = -df. \tag{89}$$

In this case, the phase spectrum $\phi_{12}(f)$ is thus a linear function of frequency with slope d, equal to the magnitude of the delay.

In general, $\phi_{12}(f)$ is a more complicated function of frequency but in view of the above example it is sensible to define the envelope or group delay

$$d(f) = -\frac{\mathrm{d}\phi_{12}}{\mathrm{d}f} \tag{90}$$

which measures the time delay between the components in the two processes at frequency f.

Turning now to the multple-taper estimates of the various functions introduces above we obviously have for the coherency estimate

$$\hat{w}_{12} = \frac{\hat{S}_{12}}{(\hat{S}_{11}\hat{S}_{22})^{1/2}} \tag{91}$$

where we have used the weighted average, (44), to estimate the auto-spectra and the estimate for the cross-spectrum is

$$\hat{S}_{12}(f) = \frac{\sum_{k=0}^{K-1} d_{1,k}(f)x_{1,k}(f)d_{2,k}(f)x^*_{2,k}(f)}{\sum_{k=0}^{K-1} d_{1,k}(f)d_{2,k}(f)}. \tag{92}$$

Here, the extra subscripts refer to the two series being analysed. The delete-one estimates, $\{\hat{w}_{(j)}\}_{j=0}^{K-1}$, used when calculating jackknife deviations, are (obviously) obtained from the above formulas by using $\hat{S}_{(j)}$ instead of $\hat{S}$ for the auto-spectra and omitting the corresponding term from the sums in (92).

The probability density of coherency estimates based on independent samples from two jointly stationary processes is complicated. Hence, it is convenient to transform this statistic so that it is approximately normally distributed. Here, the inverse hyperbolic transformation is used as suggested by Thomson & Chave (1990). We thus study

$$Q = \sqrt{2m-2}\tanh^{-1}(|\hat{w}_{12}|) \tag{93}$$

where m is the number of independent samples, which is taken as K here. (It may be more appropriate to use $v(f)/2$ from (48), and also reduce m by 1 at frequencies where line components have been removed.) The transformation (93) converts estimates of $|w_{12}|$ to an almost Gaussian distribution with mean

$$\mathrm{E}\{Q\} = \sqrt{2m-2}\tanh^{-1}(|w_{12}|) + \frac{1}{\sqrt{2m-2}} \tag{94}$$

and unit variance (Thomson & Chave, 1990). Hence, plotting the transformed coherence along with ± 1 jackknife deviation limits immediately reveals whether the jackknife tolerance is close to 1 or not.

The jackknife variance of $Q(|\hat{w}_{12}|)$ is calculated by transforming the delete-one estimates $\hat{w}_{\lceil j \rceil}$ using (93), and then proceeding in the standard way described in appendix B. If the average over frequency of the jackknife variance falls far from the predicted value of 1, some assumptions of the theoretical variance calculations are probably incorrect (e.g. the processes are non-stationary, outliers in the data, etc.).

Finally, the phase spectrum ϕ_{12} is estimated. We follow Thomson & Chave (1990) when calculating jackknife deviations. The phase is given by

$$\hat{\phi}_{12} = \frac{\hat{w}_{12}}{|\hat{w}_{12}|} \tag{95}$$

and the delete-one phase factors, $\hat{\phi}_{\lceil j \rceil}$ are calculated by substituting $\hat{w}_{\lceil j \rceil}$ in (95). The jackknife variance of $\hat{\phi}_{\lceil \cdot \rceil}$ is then given by

$$\mathrm{var}\{\hat{\phi}_{\lceil \cdot \rceil}\} = 2(m-1)(1 - |\hat{w}_{\lceil \cdot \rceil}|), \tag{96}$$

and this value is used when calculating ± 1 jackknife deviations for $\hat{\phi}_{12}$. As discussed above, the slope of the phase spectrum represents the group delay between the two processes.

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Appendix A: The mtm-program

The program developed to implement the MTM is written in C. It is written as a UNIX-filter, i.e. all interaction with the program is through parameters given on the command line and all output is to files specified there (or *stdout*). The program can be split up into three parts: processing of control parameters and input of data, spectral analysis calculations, and output of results.

A.1 Parameters and input

When the program is run without any parameters by writing

hengill:~ > mtm

(or with some unknown parameters) the following message appears:

Usage: mtm -i *infile* [*infile2*] -o *outfile* -v *dpss-file*
-w ⟨*NW*⟩ -k ⟨*K*⟩ -L -S -n ⟨*nd*⟩ -a ⟨*nm*⟩ -s ⟨*skip*⟩ -c ⟨*cp*⟩
-x ⟨*xcol*⟩ -y ⟨*ycol*⟩ -f ⟨*low*⟩ -F ⟨*hi*⟩ -d ⟨*step*⟩
i *infile* - input from *infile* (*stdin*)
o *outfile* - output to *outfile* (*stdout*)
v *dpss-file* - read/write dpss from/to *dpss-file* (/dev/null)
w ⟨*NW*⟩ - bandwidth-time value used in dpss (4)
k ⟨*K*⟩ - number of eigenspectra used (5)
L - use log(data) (no)
S - interpolate with spline (no)
n ⟨*nd*⟩ - use *nd* points of data (all)
a ⟨*nm*⟩ - use *nm*-point averages (1)
s ⟨*skip*⟩ - skip first *skip* points (0)
x ⟨*xcol*⟩ - use *xcol* as x-data from multicolumn datafile (1)
y ⟨*ycol*⟩ - use *ycol* as y-data from multicolumn datafile (2)
f ⟨*low*⟩ - lower freq. limit of spectra in units of nyquist frequency (0)
F ⟨*hi*⟩ - upper freq. limit of spectra in same units (1)
d ⟨*step*⟩ - frequency resolution for spectra in same units (1/*Nfft*)
c ⟨*cp*⟩ - critical probability for reshaping (1-1/*nd*)
t ⟨*cf*⟩ - critical F-test value for reshaping (0)
P - use point regression in reshaping (default)
I - use integral regression in reshaping (no).

Default values are quoted in parenthesis. All the the parameters are optional in the sense that the program can be run with default values by redirecting *stdin* from a datafile and redirecting *stdout* to some output file. The only requirement is that at least one option be given on the command line (otherwise only the help message is printed and the program exits). Hence, the simplest form for running the program is (-P is just included to suppress the default message)

hengill:~ > mtm -P < mydata.dat > mtm_mydata

or the equivalent form

hengill:~ > mtm -i mydata.dat -o mtm_mydata

Note that the DPSS will not be saved here since no -v option is given.

When two input files are specified, indicating that cross-spectral analysis is to be performed between the two data sets, their names have to be enclosed in quotation marks (" or '):

hengill:~ > mtm -i "mydata1.dat mydata2.dat" -o mtm_mydata

This requires that the two data sets have the same sampling rate and are of equal length. The column used as time data is selected with the -x option (defaults to 1) and the column with the time series itself is selected with the -y option (default is column 2).

The -n and -s options control which part of the original data is passed to the mapping routine. Here, the data is transformed according to the -L, -S and -a options. Note that averaging reduces the number of points by a factor of $1/nm$.

The *dpss-file* is read if it exists but otherwise it is created and the Slepian sequences calculated according to the values of N, NW and K, which are set using the -n, -w and -k option respectively, or determined from default values ($nd =$ number of data, $NW = 4$, $K = 5$). After reading (or calculating and writing) the DPSS, points where no data is available (indicated by NA in input file) are set to 0. This method of treating series with missing data is commented on in Lindberg & Park (1987). However, the theory of spectral analysis of unequally spaced time series is not very developed and this feature should be used with caution.

The -f and -F options control which part of the spectrum is written to *outfile*. The default is to write the whole spectrum, from $f = 0$ to the Nyquist frequency. The resolution of the Fourier transforms is determined from the length of the data. By default $2N \leq N_{\mathrm{FFT}} < 4N$ and the corresponding resolution is $\Delta f = 1/2N_{\mathrm{FFT}}$, but higher resolution can be requested by using the -d option. Note that values given with -f, -F and -d are in units of Nyquist frequency. The last four options listed control how the reshaping is performed, if -c $\langle cp \rangle$ is given, cp is used as a minimum value which the transformed F-test (from (69)) must acquire for removal of line components. The -t option is similar except that cf now is a minimum value of the F-test itself. The -P and -I flags are mutually exclusive and control which F-test is used when reshaping the spectrum.

The input formats currently implemented are only two, multi-column where one of the columns is the time variable, and sequential files preceeded by a header in the following format:

first line can contain anything (not read)
comment lines (optional)
format (0 or nonzero)
nd *t0* *dt*
data

If *format* $\neq$ 0 the rest of the file is read as a multi-column file. Otherwise it is assumed to contain only the time series and the values of *t0* and *dt* are used as starting time and sampling interval, while *nd* is determined from the actual number of data read.

A.2 Spectral analysis procedure

The first step in the spectrum estimation is to calculate the eigencoefficients according to (33). This is done in *mtm_eigenft* by FFT-ing the tapered series. The weights of each eigenspectrum are then calculated using the iteration procedure described in section 4.2. The subroutine *mtm_weight* takes care of this and also calculates the variance of the spectrum using the jackknife method. The jackknife variance is calculated in two ways: by jackknifing the weighted average of the eigenspectra, (44), and by jackknifing directly the iteration scheme, in which case different weights are found for each delete-one spectrum estimate. These two methods should give comparable results.

The second step is harmonic analysis. Two variants are included, point regression, where the amplitudes and F-test values are determined by (58) and (59) respectively, and integral regression where (61) and (62) are used. In practice, the formula for $\hat{\mu}_I$ is written as

$$\hat{\mu}_I(f_i) = \frac{\sum_{k=0}^{K-1} \lambda_k \sum_{t=0}^{N-1} x(t) v_k^2(t) \exp(-i2\pi f_i t)}{\sum_{k=0}^{K-1} \lambda_k} \tag{97}$$

where the sum over t is evaluated by using FFT and the f_i's are the FFT bin frequencies. The integral regression F-test values are then evaluated from

$$F_I(f_i) = \frac{(K-1)|\hat{\mu}_I(f_i)|^2 \sum_{k=0}^{K-1} \lambda_k}{\sum_{k=0}^{K-1} \int_{f=f_i-w}^{f_i+w} |x_k(f) - \hat{\mu}_I(f_i) V_k(f-f_i)|^2 \mathrm{d}f} \tag{98}$$

at the same frequencies f_i. Here, $w = 2N_{\mathrm{FFT}}W$ is the width of the windows in units of $\Delta f = 1/2N_{\mathrm{FFT}}$. Note that two degrees of freedom are assumed for line components. The integral in (98) is evaluated using the extended Simpsons rule

(Abramovitch & Stegun, 1965, formula (25.4.6)). The routines which perform the harmonic analysis are called *pr_harmonic_analysis* and *ir_harmonic_analysis*.

The next step is to reshape the spectrum. The criterion used for detection of lines is given by *cp* or *cf* as described above. New eigencoefficients, $x_k^{\mathrm{rshp}}(f_i)$ are first calculated by subtracting the lines,

$$x_k^{\mathrm{rshp}}(f_i) = x_k(f_i) - \sum_{j=0}^{J-1} \hat{\mu}(f_j^{\mathrm{line}}) V_k(f_i - f_j^{\mathrm{line}}), \tag{99}$$

where the sum is over all the J lines that reach the detection limit. The frequencies $\{f_j^{\mathrm{line}}\}_{j=0}^{J-1}$ are found by searching for local maxima in the F-test that reach above the prescribed F-test, or transformed F-test, level. The continuous spectrum is then constructed by weighting the reshaped eigencoefficients using the same iterative method as before. The final spectrum estimate is composed by superimposing the line components on the continuum, using the shape of the corresponding peaks of the F-test (see Thomson, 1990b). The routines used here are *mtm_reshape*, *mtm_weight* and *mtm_insert_lines*.

The variance of the line frequencies is calculated by jackknifing the point regression F-test, i.e. finding its maxima when each window is deleted in turn. This gives a sample of K estimates of the peak frequency and the variance is determined from this sample as described in appendix B. The relevant routines are all in the source file *jackknife.c*.

If two input files were given with the -i option the program will first process both of these as described above and write the spectral analysis results for each time series. It will then perform cross-spectral analysis, calculate the coherency, its phase and the transformed coherence as described in section 6.

A.3 Format of output

The final step in the program is output of results. For each input file the program writes two files, called *outfile.spctr* and *outfile.info*, which contain the spectral estimation results and information on the calculations respectively. The format of the *.spctr* file is as follows:

column	contents
1	frequency (usually from 0 to Nyquist = $1/2\Delta t$)
2	raw, weighted spectrum estimate (before reshaping)
3	reshaped spectrum estimate, including lines
4	weighted background spectrum estimate
5	5% confidence limit on background spectrum, from (52)
6	95% confidence limit on background spectrum, (52)
7	phase spectrum of background spectrum, from (47)
8	point regression harmonic amplitudes, equation (58)

9	point regression F-test, equation (59)
10	point regression F-test, transformed to $[0,1]$ using (69)
11	integral regression harmonic amplitudes, equation (61)
12	integral regression F-test, equation (62)
13	integral regression F-test, transformed to $[0,1]$ using (69)
14	variance of $\log(\bar{S})$, obtained by jackknifing weighted spectrum, equation (51)
15	variance of $\log(\hat{S})$, obtained by jackknifing iteration scheme, (43) and (44)
16	stability estimate of raw, weighted spectrum, from (48)
17	stability estimate of background spectrum, obtained from (48)
18	jackknife bias estimate of log(raw, weighted spectrum), (53)
19	jackknife bias estimate of log(background spectrum), from (53)

A sample *.info* file is given below. The first line gives the name of the input file. Lines 2 and 3 give the number of points, the time origin, and time interval, for the original and mapped data respectively. The variance and mean given in line 4 are deduced from the mapped data and the next two lines give the frequency range, FFT-resolution and N_{FFT}. Lines 7 and 8 give bias and variance estimates of $\log S$ deduced from Gaussian theory with $\nu = 2m$ being the degrees of freedom of the spectrum estimate. The bias estimate is

$$B_\chi(m) = \psi(m) - \log m, \tag{100}$$

and the variance of $\log S$ is given by

$$\mathrm{var}(\log S) = \psi'(m) \tag{101}$$

where ψ is the digamma function and ψ' the trigamma function. Formulas for computing ψ and ψ' can be found in Abramowitz and Stegun (1965). These values are to be compared with the jackknife estimates in columns 14 and 18 in the *.spctr* file. Significant departures from the Gaussian values can indicate outliers or nonstationarity (see Thomson & Chave, 1990, and Thomson, 1990b, for details).

The Rayleigh resolution and bandwidth of filters is listed along with the total variance and variance in lines as estimated from (42). The innovations variance for the background spectrum is given in units of the variance of the continuum:

$$\sigma_I^2 = \frac{1}{\hat{\sigma}_c^2} \exp\left(\int_{-1/2}^{1/2} \log(\hat{S}_c(f)) \mathrm{d}f \right) \tag{102}$$

with

$$\hat{\sigma}_c^2 = \int_{-1/2}^{1/2} \hat{S}_c(f) \mathrm{d}f \tag{103}$$

being the continuum variance. The properties of the DPSS are next, with the average variance efficiency derived from the K sequences used being

$$\Xi_K = \frac{1}{N \sum_{t=0}^{N-1} \left[\frac{1}{K} \sum_{k=0}^{K-1} v_k^2(t) \right]^2}. \tag{104}$$

Thomson (1982) comments on variance efficiency and emphasizes that it should not be taken as a strong criterion when comparing spectrum estimates since it is strictly only valid for white noise processes and also ignores bias.

The last part of the *.info* file lists the properties of the line components that have been removed from the initial raw spectrum. The first column gives the frequency of the maxima in F-test, the jackknife estimate is in column two and the jackknife standard deviation in the third one. The period and estimated standard deviation are given along with amplitude and phase, determined from (58) or (61) as selected with the -P/-I options. The final column is the F-test value at the frequency in column 1.

```
# Infile: hiti6001-8410.030
# In: points = 298     t0 = 85      dt = 1
# Map: points = 298    t0 = 85      dt = 1
#   variance = 98.9531     mean = -56.2855
# Spectra: low f = 0   high f = 0.5    df = 0.000488281    dt = 1
#   nfft = 1024
# Gaussian bias of lnS,     Psi(5)-ln5 = -0.10332  Psi(4)-ln4 = -0.130177
# Gaussian variance of lnS, Psi'(5) = 0.221323     Psi'(4) = 0.283823
# Rayleigh resolution, 1/N = 0.0033557    4/N window = 0.0134228
# Estimated total variance, sigma^2 = 3289.07
# Estimated variance in lines, sigma^2-sigmar^2 = 3277.16
# Innovations variance, (sigmai/sigmar)^2 = 0.828152
# DPSS: points = 298    NW = 4    K = 5    VarEff = 0.816485
# 2 lines above 0.996644 ftest confidence level, integral regression
# freq.    jackf      df          period T  dT        amplitude  phase    F-test
0.0834961  0.0834961  0.00142494  11.9766   0.204392  13.3767    1.48245  592.713
0          0          0.00113242  ++        ++        56.4594    1.5708   33.4898
```

A sample *.info* file.

When cross-spectral analysis is performed the program writes similar files for the second input file, called *outfile2.spctr* and *outfile2.info*. It also creates a separate file, *outfile.csa*, with the cross-spectral analysis results in the format given below:

column	contents
1	frequency (usually from 0 to Nyquist = $1/2\Delta t$)
2	magnitude squared coherence, $\lvert\hat{w}_{12}\rvert^2$ from equation (91)
3	normal transform of coherence, $Q(\hat{w}_{12})$ given by (93)
4	$Q(\hat{w}_{12}) - 1$ jackknife deviation
5	$Q(\hat{w}_{12}) + 1$ jackknife deviation
6	phase of coherency, $\hat{\phi}_{12}(f)$ from equation (95)
7	$\hat{\phi}_{12}(f) - 1$ jackknife deviation, equation (96)
8	$\hat{\phi}_{12}(f) + 1$ jackknife deviation, equation (96)

A.4 Some comments on additions

All dynamic allocation of data structures is contained in *alloc.c*. The data-structures are defined in the header file *fastar.h* and extending them is simply done by adding the required components to the structures and allocating space in the corresponding *alloc*-routines. Remember also to change the relevant *free*-routines.

Since the main emphasis here has been on the analysis of short time series, section averaging has not been incorporated into the current program but this should not be difficult (see Thomson & Chave, 1990). Robustification of the section-averaging method is also well documented in the literature and gives superior results to standard techniques when the data is contaminated with outliers (Chave *et al.*, 1987; Thomson & Chave, 1990; see also Thomson, 1977).

The next addition to the mtm-program will be the coding of the multiple-line test, described by Thomson (1990b). This is a necessary tool to detect line components that are separated by less than the filter bandwidth.

One further refinement that needs consideration is to apply the bootstrap method to determine confidence levels for the integral regression F-test (Lindberg & Park, 1987). In the meantime, it is probably better to use the point regression F-test, since its distribution is closer to the true F-distribution.

Appendix B: A few statistical terms

In this report, most of the statistical terms have been used without further definition. Below, some of these are defined, and the jackknifing method is described.

The set of points representing the possible outcomes of an experiment defines the sample space of the experiment. A random variable is a real (or complex) valued function defined on this space. The probability density, ρ, of a continuous random variable x is defined by the following properties:

(i) $\rho(x) \geq 0$
(ii) $\int_{-\infty}^{\infty} \rho(x)\mathrm{d}x = 1$
(iii) $\int_a^b \rho(x)\mathrm{d}x = P(a < x < b)$

where $P(\cdot)$ denotes probability. We are often interested in some parameters of the density function, $\rho(x)$, e.g. the mean and variance of the random variable x which are given by the first and second moments of the density respectively. The distribution function, F, of the continuous random variable x is given by the integral of the density:

$$F(X) = \int_{-\infty}^{X} f(t)\mathrm{d}t = P(x \leq X). \tag{105}$$

Consider a random variable x whose density fuction depends on the parameter θ. Let $x_1, \ldots, x_N$ represent a random sample of n independent observations of

x and let $\hat{\theta}(x_1, \ldots, x_N)$ be a function of the sample that is taken as an estimate of θ. Such a function is called a statistic. It is said to be sufficient if it can be inverted to obtain the original data. A statistic is a random variable whose value is determined solely by the sample values. A statistic $\hat{\theta}(x_1, \ldots, x_N)$ is called an unbiased estimate of the parameter θ if $\mathrm{E}\{\hat{\theta}\} = \theta$ for all θ. This means that the distribution of the random variable $\hat{\theta}$ has the mean value θ (see, e.g. Hoel, 1971).

Now, denote by $\hat{\theta}_{\text{all}}$ the estimate of θ obtained by using all the N observations available, then form N additional estimates, $\{\hat{\theta}_{\lceil i \rceil}\}_{i=1}^{N}$, by deleting each observation in turn from the sample, i.e.

$$\hat{\theta}_{\lceil i \rceil} = \hat{\theta}(x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_N). \tag{106}$$

These values are termed delete-one estimates and are the key ingredients in the jackknifing method. Although the jackknife was first introduced to obtain a lower bias estimate of $\hat{\theta}_{\text{all}}$, a more important application for it is in the nonparametric estimation of the variance of an arbitrary statistic. The jackknife variance of $\hat{\theta}_{\text{all}}$ is given by (Thomson & Chave, 1990)

$$\mathrm{var}\{\hat{\theta}_{\text{all}}\} = \frac{N-1}{N} \sum_{i=1}^{N} \left[\hat{\theta}_{\lceil i \rceil} - \theta_{\lceil \cdot \rceil}\right]^2 \tag{107}$$

where

$$\theta_{\lceil \cdot \rceil} = \frac{1}{N} \sum_{i=1}^{N} \hat{\theta}_{\lceil i \rceil} \tag{108}$$

is the mean of the delete-one estimates.

The statistical properties of the jackknife are discussed in Thomson & Chave (1990). It is emphasized that transforming the random variable being jackknifed is essential when its distribution is bounded or strongly non-Gaussian. The transformations used above are the logarithmic transformation when jackknifing power spectra and the inverse hyperbolic transformation when jackknifing coherences.

The notion of mean-square convergence is defined as follows (Priestley, 1981):
Definition: Let $U_1, U_2, \ldots, U_i, \ldots,$ be a sequence of random variables. The sequence $\{U_i\}$ converges in mean square if and only if there exists a random variable U such that

$$\lim_{i \to \infty} \mathrm{E}\{(U_i - U)\} \quad = \quad 0.$$

This is denoted by

$$\underset{i \to \infty}{\text{l.i.m.}}\, U_i = U. \tag{109}$$

The Riemann-Stieltjes integral of the form

$$\int_a^b g(t) \mathrm{d}Z(t)$$

is then defined as the mean-square limit of the discrete summation

$$\sum_{i=1}^{n} g(t_i)\{Z(t_i) - Z(t_{i-1})\}.$$

A very extensive discussion on orthogonal increment processes is given in Priestley (1981, ch. 4). Here we only restate the fundamental theorem which states that every stationary process can be expressed in terms of such a process. **Theorem:** Let $\{X(t)\}, -\infty < t < \infty$, be a zero-mean stochastically continuous stationary process. Then there exists an orthogonal process, $\{Z(\omega)\}$, such that, for all t, $X(t)$ may be written in the form,

$$X(t) = \int_{-\infty}^{\infty} \exp(i\omega t)\mathrm{d}Z(\omega), \tag{110}$$

the integral being defined in the mean-square sense. The process $\{Z(\omega)\}$ has the following properties:

(i) $\mathrm{E}\{\mathrm{d}Z(\omega)\} = 0$ for all ω
(ii) $\{|\mathrm{d}Z(\omega)|^2\} = \mathrm{d}H(\omega)$ for all ω
where $H(\omega)$ is the (non-normalized) integrated spectrum of $X(t)$.
(iii) for any two distinct frequencies, $\omega, \omega', (\omega \neq \omega')$
$\mathrm{E}\{\mathrm{d}Z^*(\omega)\mathrm{d}Z(\omega')\} = 0$.

The results of this theorem carry over to the discrete case, the only modification being that the range of the integration becomes $(-\pi, \pi)$ and the condition that the process be stochastically continuous is no longer meaningful. The result is the spectral representation (5), where we have used frequency f instead of angular frequency $\omega = 2\pi f$.