A C-SUBROUTINE FOR COMPUTING MULTIPLE-TAPER SPECTRAL ANALYSIS

JONATHAN M. LEES AND JEFFREY PARK
Dept. of Geology and Geophysics, Yale University
PO Box 208109, New Haven CT 06520-8109
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Abstract

A simple set of subroutines in ANSI-C are presented for multiple taper spectrum estimation. The multitaper approach provides an optimal spectrum estimate by minimizing spectral leakage while reducing the variance of the estimate by averaging orthogonal eigenspectrum estimates. The orthogonal tapers are Slepian $n\pi$ prolate functions used as tapers on the windowed time series. Since the taper functions are orthogonal, combining them to achieve an average spectrum does not introduce spurious correlations as standard smoothed single-taper estimates do. Furthermore, estimates of the degrees of freedom and F-test values at each frequency provide diagnostics for determining levels of confidence in narrow band (single frequency) periodicities. The program provided is portable and has been tested on both Unix and Macintosh systems.

Introduction

Accurate estimation of the spectra of geological and geophysical time series is becoming increasingly important as researchers seek narrow band correlations of disparate data series. A similar problem arises when we need to isolate single frequencies embedded in white noise or some other continuous background spectrum. Examples include such diverse fields as the study of free oscilations of the earth (Park, et al., 1987a, Lindberg and Park, 1987) and the correlation of long term geological data sets with Milankovich astronomical cycles (Thomson, 1990; Berger et al, 1991; Park and

Maasch, 1993). Numerous texts have been written on this subject and difficulties involved in estimating a power spectrum with both good leakage properties and low variance is a subject of intense investigation, see for example Kay and Marple (1981) . The traditional single taper analysis has the objectionable feature that portions of the time series are excluded from analysis as a trade-off for reducing spectral leakage in the frequency domain. Park et al. (1987b) demonstrate that smooth spectrum estimates using Slepian tapers avoid this tradeoff.

In this paper we present a portable subroutine for calculating a multitaper spectrum estimate for a geophysical or geological time series. Multitaper analysis arises as an extension of traditional taper analysis where time series (or auto-correlation functions) are tapered prior to Fourier transform to reduce bias due to leakage. Common single taper methods include applying Hann, 20% cosine or numerous other tapers, which reduce the effects of spectral leakage. In the multitaper approach an orthonormal sequence of tapers is designed to minimize spectral leakage. The set of tapers and the associated eigenspectra can be combined to reduce the variance of the overall spectrum estimate. One of the main advantages of the multitaper spectrum estimates is that formal estimates of their statistical degrees of freedom and variance are simple consequences of the procedure. Alternatively, nonparametric jackknife estimates of variance in spectrum and coherence estimates are easily implemented (Thomson and Chave, 1989; Vernon et al, 1991). In addition, the algorithm includes an F-test which can be used to identify the location and confidence bounds of spectral peaks presumed to represent periodic, phase-coherent signals (Thomson, 1982).

An optimal choice of tapers was derived (Slepian (1978), see Slepian (1983) for a review) in an effort to identify optimally bandlimited functions for finite time intervals. These functions are called $p\pi$-prolate functions. A simple algorithm for determining them is given below. After they are applied to the data window, the fast Fourier transform (FFT) is applied individually to each tapered estimate. The resulting "eigenspectra" are combined to form the final estimate. The steps are outlined briefly below.

1 Algorithmic Steps

The algorithm calculates $NWIN$ $p\pi$-prolate Slepian tapers for a given series length N, tapers the data series, applies the fast Fourier transform to each of $NWIN$ tapered copies of the data, and then averages the weighted Fourier transforms to achive a high-resolution low-variance spectrum estimate. The analysis is described in detail in Percival and Walden (1993) , p. 386-387, and parts of the algorithm are discussed by Thomson (1982) and Park, et al. (1987abc) . First, a tridiagonal matrix is formed by calculating diagonal elements,

$$([N-1-2n]/2)^2 \cos(2\pi p/N), \qquad n = 0, ..., N-1 \tag{1}$$

and off diagonal elements

$$n(N-n)/2, \qquad n = 0, ..., N-1 \tag{2}$$

The "time-bandwidth" product p scales the frequency band over which the tapers average spectral information – its halfwidth is $f_w = p/T$, where T is the duration of the time series.

We have used the EISPACK routines *tridib* and *tinvit* to solve for the eigenvalues and eigenvectors of the tridiagonal system. To keep the program entirely in C, in our implementation we translated the EISPACK routines to C using the public domain software *f2c* available over the internet, although these two routines are not very complicated and can be easily translated to C directly. The $NWIN$ eigenvectors form the taper functions which are applied to the time series sequentially prior to Fourier transformation. An example of 3π-prolate Slepian tapers (NPI=3) is presented in Figure 1 with $NWIN = 5$. Notice that the first eigenfunction (solid line) looks like a typical single taper. The higher-order tapers have several zero crossings and weigh the data near the ends more heavily. Since the eigenvectors are orthogonal they represent mutually orthogonal functions in both the time and frequency domains. They are also mutually orthogonal in a narrow frequency range around the estimation frequency f_o. Because of this property in the frequency domain, spectrum estimates from the differently tapered data series can be combined without inducing correlations, either for purely white data processes or for "locally white" data processes (i.e. cases where the spectrum is smoothly varying).

The output of the discrete Fourier transform of an N-point data series x_n with the kth Slepian taper $w_n^{(k)}$ is a complexed-valued "eigenspectrum" $Y_k(f)$, where

$$Y_k(f) = \sum_{n=1}^{N} w_n^{(k)} x_n e^{i2\pi f n \Delta t} \tag{3}$$

where Δt is the sampling interval of the time series. Many applications normalize $Y_k(f)$ by dividing (3) by N, $N\Delta t$, or $\sqrt{N}$. In practice, the tapered data arrays are zero-padded to the next higher power of 2 in preparation for the FFT, so that the discrete Fourier transform (DFT) is calculated only at discrete values of frequency f. We have used the routine *realft* from Numerical Recipes (Press, et al., 1986) to calculate the FFT of the real-valued tapered data series. Any FFT routine can be substituted in place of *realft* if the user does not have access to it. The $NWIN$ individual spectra are then combined to achieve the final spectrum estimate. Padding to a larger power of two interpolates the spectrum estimator, which may make visual assessment easier.

We have provided two subroutines for the combination of the eigenspectra. The first, called *hires*, averages the eigenspectra weighted according to respective eigenvalues:

$$S(f) = \sqrt{\sum_{k=0}^{NWIN-1} (\lambda_k N)^{-1} \left|Y_k(f)\right|^2} \tag{4}$$

where $|Y_k|^2$ is the squared modulus of the corresponding eigenspectra. λ_k is the "bandwidth retention factor" which specify the proportion of narrow-band spectral energy captured by the kth Slepian taper for a white-noise process. $\lambda_k \approx 1$ for tapers that possess good resistance to spectral leakage. This is an optimal choice of weights when estimating pure white noise. The second, "adaptive" spectrum estimator, appropriate for a colored spectrum, is calculated in routine *adwait*. It seeks an optimal set of weights which minimizes the misfit of the estimated spectrum to the true spectrum, using the bandwidth retention factors to estimate the uncertainty of each "eigenspectrum" $Y_k(f)$. The algorithm is iterative and usually converges after only a small number of trials. To start, we take the average of the $k = 0$ and $k = 1$

eigenspectra to estimate the true spectrum $S(f)$. The optimal weights d_k are given by the formula,

$$d_k(f) = \frac{\sqrt{\lambda_k} S(f)}{\lambda_k S(f) + \sigma^2 (1 - \lambda_k)} \tag{5}$$

where $\sigma^2 = \sum_{n=1}^{N} x_n^2$ is the process variance of the data series.

Using these weights, new estimates of $S(f)$ are derived and new weights calculated recursively with the previous $S(f)$ estimates until the process converges to within a given tolerance. The adaptive weights provide an optimal balance between spectral leakage resistance and spectrum estimation variance that varies as a function of frequency f.

2 Confidence Test For Periodicity

The confidence test for a periodic, phase-coherent signal is measured with an F variance-ratio test. An F-test compares the variance explained by a model for data versus the residual variance that the model fails to predict. The linear regression for the complex amplitude of a suspected periodic signal, as well as the F-test formula, are derived by Thomson (eq. 13.10) and discussed by Park et al. (1987a) and Percival and Walden (1993, p. 499). The amplitude $C(f_1)$ of a phase-coherent sinusoid at frequency f_1 is estimated by a regression over eigenspectra $Y_k(f_1)$, leading to the formula

$$C(f_1) = \frac{\sum_{k=0}^{NWIN-1} W_k^*(0) Y_k(f_1)}{\sum_{k=0}^{NWIN-1} |W_k(0)|^2} \tag{6}$$

where $W_k(f)$ is the discrete Fourier transform of the kth $p\pi$-taper and the asterisk denotes complex conjugation. Note that $W_k(0)$ is real-valued. The F-test at frequency f_1 is a weighted ratio of the variance explained by a phase-coherent model for the eigenspectra $Y_k(f_1)$ versus the residual variance:

$$\frac{(NWIN-1)|C(f_1)|^2 \sum_{k=0}^{NWIN-1} |W_k(0)|^2}{\sum_{k=0}^{NWIN-1} |Y_k(f_1) - C(f_1)W_k(0)|^2} \tag{7}$$

In subroutine *get_F_values* the real and imaginary components of $C(f)$ are denoted *amur* and *amui*.

3 Examples

Here we provide simple examples for illustration. There are several more technical examples discussed in the references. In the first example we consider is a simple sinusoid with 2 frequencies at $f_1 = 20$ Hz and $f_2 = 30$ Hz (Figure 2),

$$y(t) = 2.0 * \sin(2\pi f_1 t) + 3.0 * \sin(2\pi f_2 t) + noise$$

where $t = n\Delta t$ is the discrete time (Figure 2). We expect to see two peaks in the frequency domain. These are smoothed over an interval with halfbandwidth $f_w = p/(N\Delta t)$. For comparison purposes, we use this smoothing window when computing the smoothed naive spectrum. The multi-taper spectrum is presented in Figure 3 along with the smoothed single taper estimate and an autoregressive estimate using 40 coefficients (AR(40)). The multitaper estimate is comparable to the AR(40) in terms of the variance although the AR(40) appears to have slightly higher variance in the high frequency range. The single taper estimate has considerably more variance, and sharper peaks at the 20 and 30 Hz singlets than the multitaper estimate. The degrees of freedom for the multitaper estimate are presented in figure 4a along with the F-test values in figure 4b. Note the sharp peaks ($>$ 99%confidence for nonrandomness) at 20 and 30 Hz in the F-test display. These can be used to reshape the spectrum by a technique suggested by Thomson (1982) and explained in detail in Percival and Walden, p. 512-513.

As a second test we apply these methods to a time series which has some relevance to earthquake source analysis. We created a synthetic time series by summing sinc functions with random amplitudes, time shifted by one sample each for 1000 time shifts (Figure 5). Each of the sinc functions has an identical power spectrum adjusted to have a cut off at 0.125 Hz, for $\Delta t = 1$ second. The difference between subsequent signals lies in the phase spectrum. The power spectra of the ensemble is a rectangle function with corner frequency 0.125 Hz. A comparison of three estimates of the power spectrum is presented in the adjacent figure. Note that the single taper (20% cosine) spectrum does not exhibit the sharp corner frequency expected. The multitaper estimate and the autoregressive AR(120) estimate each appear to estimate the shape of the spectrum quite well (Figure 6). The MT estimate has lower variance in the lower frequency range, where all eigenspectra contribute. It has higher variance in the higher frequency range, where only the most leakage-resistant eigenspectra are retained. The F-test (Figure 7) again isolates the band of the signal that appears phase-coherent at high confidence.

In a last example we consider the time series of δ^{18}O (Park and Maasch, 1993), oxygen isotopes determined from ocean-sediment drill cores and sampled at $\Delta t = 3000$ years (Figure 8). We can identify spectral peaks at periods of 41.2, 23.7, 22.4 and 18.9 thousand years (Figure 9a). These climate periodicities are associated with the obliquity of the Earth's orbit and to the precession of the equinoxes, each of which redistributes the solar energy received by the Earth over its surface and within the annual cycle. The high F-values (Figure 9b) indicate that the corresponding spectral peaks are significantly phase-coherent, with relatively modest variation in amplitude and phase. There are also several high F-values in the high end of the spectrum. Additional scrutiny might reveal them to have a deterministic cause, for instance, the peak frequency might correlate with the time scale of a hitherto unexamined climate factor. However, since there are no peaks in the spectrum at these frequencies we regard such high F-values as likely due to random noise fluctuations. Thomson points out that there is a finite probability that sampling peculiarities will give rise to high values of significance. He suggests that F-tests at unexpected frequencies which have probabilties greater than 1-1/n, where n is the number of points in the sample, be considered significant. The δ^{18}O series in the example have $N \approx 750$, so this requirement discards F values with less than $\approx 99.8\%$ confidence for nonrandomness.

4 Implementation

The program is set up to be modular, so that different parts can be used without employing the whole program. A driver program handles the I/O of the input signal and produces a file containing all the relevant statistics and estimates presented in the figures above. Thus the subroutines that analyze the spectrum can be extracted and embedded in other analysis code. The code below is set up to read a data stream with appropriate parameters, apply the multitaper analysis and dump out the results. If the code will be used to calculate many spectra with the same number of data points (same window length), then the calculation of the taper weights (subroutine *multitap*) can be executed once and the tapers may be applied repeatedly on the different incoming data streams. This can be achieved with a slight re-organization of the *do_mtap_spec* routine.

We have implemented this code on a Sun Sparc-2 using the Gnu C compiler, gcc. We also transported the code, with some minor modification, to a Macintosh-IIsi and compiled it with Think Technologies, Think C. The program runs considerably faster on the Sparc-2, but even on the Mac the clock time was not unreasonable (several seconds). For simple spectral analysis the added information (the degrees of freedom and the F-test) provided by the multi-taper code should compensate for the additional computational effort. The code is presented below in a fashion that is easy to understand and modify and has not been optimized for memory efficiency or speed. Undoubtedly, a small amount of effort may increase these efficiencies a considerable amount.

This code is available via anonymous ftp from milne.geology.yale.edu.

5 References

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6 Figure Captions

Fig. 1: $p\pi$-prolate functions for $p = 3$ and $NWIN = 5$. Note that the low order function (1) is similar to typical single taper functions. As the order increases the ends are weighted more heavily in the spectrum estimation.

Fig. 2: Example synthetic time series with 2 sinusoidal components at $f_1 = 20$ Hz and $f_2 = 30$ Hz plus additive noise.

Fig. 3: Comparison of multitaper, single taper, and autoregressive estimates of the signal in Figure 2. Frequency is scaled as fractions of the sampling frequency from 0 to Nyquist. Note the peaks at $f_1 = 20$ Hz and $f_2 = 30$ Hz

Fig 4: (a) Estimates of the effective degrees of freedom for the multitaper spectrum presented in figure 3. The width of the peaks at the two sinusoidal frequencies illustrates the smoothing window for the spectrum estimations. (b) F-test values for the multitaper spectrum presented in figure 3. Horizontal lines represent levels of 99, 98, 95, and 90% confidence with 2 and 8 degrees of freedom. The narrow band delineation of the single frequency signals in the F-test can be used to reshape the spectrum.

Fig. 5: Synthetic time series composed of 1000 sinc functions with random amplitude and linear phase shift. Each sinc function posesses the same amplitude spectrum and differ randomly only in their respective phase.

Fig. 6: Comparison of multitaper, single taper, and autoregressive estimates of the signal in Figure 5. The bias of the single taper estimate is clearly evident. The difference between the autoregressive estimate and the multitaper estimate is small.

Fig 7: (a) Estimates of the effective degrees of freedom for the multitaper spectrum presented in figure 5. (b) F-test values for the multitaper spectrum presented in figure 5. Horizontal lines represent levels of 99, 98, 95, and 90% confidence with 2 and 8 degrees of freedom. Note how the degrees of freedom and the F-test allow for a quick assessment of the periodic or quasiperiodic nature of spectral peaks.

Fig. 8: δ^{18}O time series from a drill core with sampling interval $\Delta t = 3000$ years

taken from δ^{18}O (Park and Maasch, 1993). The δ^{18}O data are measured on oxygen isotopes determined from ocean-sediments. Signals in this time series provide important constraints on models of past climatic change.

Fig. 9: Comparison of multitaper, single taper, and autoregressive estimates of the signal in Figure 8. Narrow band signals which show a high correlation with time series related to orbital periodicities are marked and discussed in the text.

Fig 10: (a) Estimates of the effective degrees of freedom for the multitaper spectrum presented in figure 9. (b) F-test values for the multitaper spectrum presented in figure 9. Horizontal lines represent levels of 99, 98, 95, and 90% confidence with 2 and 8 degrees of freedom. Only signal with periods that have high F-test and high spectrum amplitude are considered significant and warrant serious interpretation.