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**BASIC ELEMENTS OF POWER SPECTRAL
ANALYSIS**

Davis D. Sentman

Iowa University

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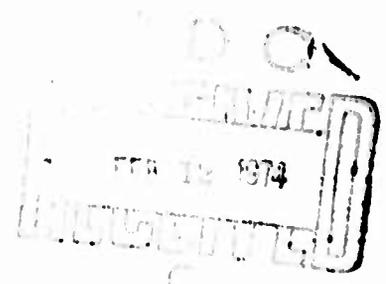
BASIC ELEMENTS OF POWER SPECTRAL ANALYSIS*

by

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January 1974



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PREFACE

This report is intended to be a brief summary of the most basic elements of the subject of Power Spectral Analysis of time-series data. These elements are presented and discussed heuristically without rigorous mathematical justification. It is hoped that the material may be used as a practical reference for those gaining their first exposure to the subject, although key references are given for further research into specific points. Any errors of omission most likely reflect the author's limited exposure to the field through his application of the method to a few particular research problems.

ABSTRACT

A short presentation is made on the basic elements of Power Spectral Analysis with emphasis on the Blackman-Tukey method. Short discussions are included on the topics of pre-whitening, frequency and spectral windows, and statistical reliability. Examples are included whenever possible, and a Fortran subroutine for calculating a power spectrum is presented.

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TABLE OF CONTENTS

	Page
I. BRIEF BACKGROUND	1
A. Historical Roots	1
B. Ergodicity and Stationarity	1
C. Notation	2
1. Fourier Transform	3
2. Correlation Functions	3
a. Convolution	3
b. Cross Correlation	4
c. Autocorrelation	4
II. THE POWER SPECTRUM FOR THE CONTINUOUS CASE	6
III. FINITE DATA SETS	10
A. Effect of Data Truncation on the Power Spectrum	10
B. Reducing Frequency Window Leakage	13
1. Data Tapering	13
2. Tapering the Autocorrelation Function	15
3. Pre-whitening	20
IV. DIGITIZED DATA	26
A. Discrete Forms of Relevant Equations	26
1. MLP Method	26
2. FFT Method	30

TABLE OF CONTENTS (cont.)

	Page
B. The Statistical Reliability of the PSD Estimates . . .	34
1. Confidence Limits	34
2. k for the MLP Calculation	36
3. k for the FFT Calculation	37
C. Planning Considerations	37
1. Choosing $\Delta\tau$ and f_{\max}	38
2. Choosing M and Δf	39
D. Averaging Power Spectra	41
1. Averaged Power Spectra from Data Sets of Equal Lengths	42 42
2. Averaged Power Spectra from Data Sets of Different Lengths	43 43
V. AN EXAMPLE OF A POWER SPECTRUM CALCULATION	45
FIGURE CAPTIONS	47
APPENDIX I: A FORTRAN SUBROUTINE FOR CALCULATING POWER SPECTRA	52 52
A. Subroutine Arguments	53
B. Subroutine	54
LIST OF REFERENCES	56

I. BRIEF BACKGROUND

A. Historical Roots

Power spectral analysis is one small area of the much broader field of Communications Theory. This broader field is an indispensable part of communications engineering and provides the theoretical foundations for the design and analysis of much of the advanced engineering found in modern communications systems (Lee, 1960). The theory is basically a statistical theory in which the central idea is that noise and messages are considered to be random phenomena. Probability theory is therefore incorporated into the very foundation of the theory and is an integral part of it.

The basis of the theory finds its roots in statistical mechanics. The equivalence of time and ensemble averages, first assumed by Gibbs and later stated more precisely by Maxwell in his ergodic hypothesis, is the starting point for statistical communications theory. From this and the quasi-ergodic hypothesis are derived the formal proofs necessary for the logical development of the subject.

B. Ergodicity and Stationarity

Two conditions necessary for the development of the theory are imposed on the random ensembles of data which we wish to power spectrum analyze. We shall merely state them as being the foundation for the development of the theory, with proofs and implications to be found elsewhere.

(1) Ergodicity. The ergodic theorem may be stated as "in a stationary ensemble of random functions having a continuous range of possible values the amplitudes of an ensemble member will come infinitely close to every point of the continuous range of possible values if given an infinite amount of time." This theorem allows the replacement of ensemble averages with time averages, and is the basis for the formal analysis of communications theory.

(2) Stationarity. If the amplitude probability density of an ensemble is time independent, the ensemble is said to be stationary. In practical terms related to power spectral analysis this means that the power spectrum of a finite data set is time independent.

In addition to the two above conditions, it is assumed that the random process is Gaussian or nearly Gaussian in character, that is, the probability distribution of the elements in an ensemble is Gaussian or nearly so. Blackman and Tukey (1958) show that for an infinite data set a Gaussian assumption yields exact results, and rather good approximations otherwise.

C. Notation

With these preliminaries stated, we now give the notation to be used throughout the rest of this section. Fourier transforms, correlations (auto- and cross-), and convolutions are used rather frequently in power spectrum work. Therefore to reduce the complexity of the equations in the following discussion a simplified notation will be adopted as follows:

1. Fourier Transform

Let $f(t)$ be specified on the interval $(-\infty, \infty)$. Then define the Fourier transform

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t) e^{-i\omega t} dt .$$

We shall also use the Fourier transform operator \mathcal{F} , e.g.,

$$\mathcal{F}[f(t)] = F(\omega)$$

and inverse Fourier transform operator

$$\mathcal{F}^{-1}[F(\omega)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(\omega) e^{i\omega t} d\omega .$$

2. Correlation Functions

Let $f_1(t)$ and $f_2(t)$ be specified on the interval $(-\infty, \infty)$. We then use the following notation:

a. Convolution. Define

$$\psi_{12}(\tau) \equiv \lim_{T \rightarrow \infty} \frac{1}{T} \int_{-T/2}^{T/2} f_1(t) f_2(\tau - t) dt$$

$$\equiv f_1(t) * f_2(t)$$

where * denotes convolution.

b. Cross Correlation. Define

$$\varphi_{12}(\tau) \equiv \lim_{T \rightarrow \infty} \frac{1}{T} \int_{-T/2}^{T/2} f_1(t) f_2(t + \tau) dt$$

$$\equiv f_1(t) * f_2(-t) \quad .$$

c. Autocorrelation. Cross correlation of a function with itself. Define

$$\varphi_{11}(\tau) \equiv \lim_{T \rightarrow \infty} \frac{1}{T} \int_{-T/2}^{T/2} f_1(t) f_1(t + \tau) dt$$

$$= f_1(t) * f_1(-t)$$

$$= f_1(t) * f_1(t) \quad ,$$

the last step being a result of the symmetry of the autocorrelation operation.

In general, then, small letters will denote functions of time and capital letters Fourier transforms (functions of frequency) of the corresponding functions of time. Letters written in script will be used to denote operators. Additionally, MLP will be used as an

abbreviation for mean-lagged-product, and FFT for fast-Fourier-transform. The term "power-spectral-density" (PSD) will also be used synonymously with "power spectrum".

II. THE POWER SPECTRUM FOR THE CONTINUOUS CASE

A Fourier series is one set of orthogonal functions that may be used to expand a well-behaved function on the interval $(-\infty, \infty)$. If we consider a time series $f(t)$, we can represent it by

$$f(t) = \mathcal{F}^{-1}[F(\omega)]$$

where

$$F(\omega) = \mathcal{F}[f(t)] \quad .$$

The power spectrum of a function is defined as the absolute value squared of the Fourier transform of the function. If $P(\omega)$ is the power spectrum, then

$$P(\omega) = |\mathcal{F}[f(t)]|^2 = |F(\omega)|^2 \quad .$$

But because of the convolution theorem, which states that for two functions f_1 and f_2 ,

$$\mathcal{F}[f_1 * f_2] = F_1 \cdot F_2$$

By setting $f_1 = f_2$ we have

$$\mathfrak{F}[f_1 * f_1] = F_1 \cdot F_1 \quad . \quad (2)$$

Now $f_1 * f_1$ is the autocorrelation function for f_1 . The autocorrelation function is always an even function, i.e.,

$$f_1(t) * f_1(-t) = f_1(t) * f_1(t)$$

so that there are no sine components in its Fourier transform. The transform is therefore real and

$$\begin{aligned} \mathfrak{F}[f_1 * f_1] &= \mathfrak{F}[\phi_{11}] = \phi_{11} \\ &= F_1 F_1 = |F_1|^2 \end{aligned} \quad (3)$$

so that

$$P(\omega) = |F(\omega)|^2 \quad . \quad (4)$$

Therefore

$$P(\omega) = \Phi(\omega) = \mathfrak{F}[\varphi_{11}(t)] \quad (5)$$

or

$$|F(\omega)|^2 = \Phi_{11}(\omega) \quad (6)$$

This equality is known as the Wiener Theorem and states that the power spectrum of a time series is equal to

- (a) the Fourier transform squared of the function, or
- (b) the Fourier transform of the autocorrelation function.

It may be noted that in (a) the Fourier transform utilizes both sine and cosine terms, while in (b) the Fourier transform of the autocorrelation function has only non-zero cosine terms, that is,

$$\begin{aligned} \Phi_{11}(\omega) &= \mathfrak{F}[\varphi_{11}(t)] \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \varphi_{11}(t) \cos \omega t \, dt \\ &= \frac{2}{\sqrt{2\pi}} \int_0^{\infty} \varphi_{11}(t) \cos \omega t \, dt \quad (7) \end{aligned}$$

The first method of computing the power spectrum is the most direct and straightforward way. The fast-Fourier-transform (FFT) calculation utilizes the definition of the power spectrum directly to compute the power spectrum. The second method is known as the mean-lagged-product (MLP) method, and is the one utilized by Blackman and Tukey (1958) to calculate power spectra.

III. FINITE DATA SETS

A. Effect of Data Truncation on the Power Spectrum

The definition of the power spectrum was made for infinitely long, continuous data sets. Practical data analysis, however, requires the use of considerably less data. To determine the effects on the power spectrum resulting from the truncation of a data set to finite lengths, consider the function $f(t)$ defined on the interval $(-\infty, \infty)$ as shown in Figure 1.

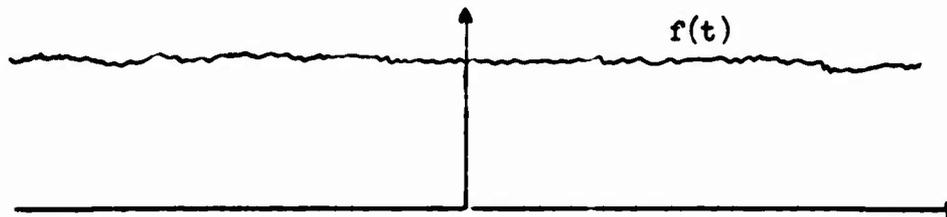


Figure 1

If we truncate $f(t)$ by multiplying by a data window $g(t)$ such that

$$g(t) = \begin{cases} 1, & |t| \leq T/2 \\ 0, & |t| > T/2 \end{cases}$$

the truncated data set becomes

$$h(t) = f(t) g(t)$$

as shown in Figure 2.

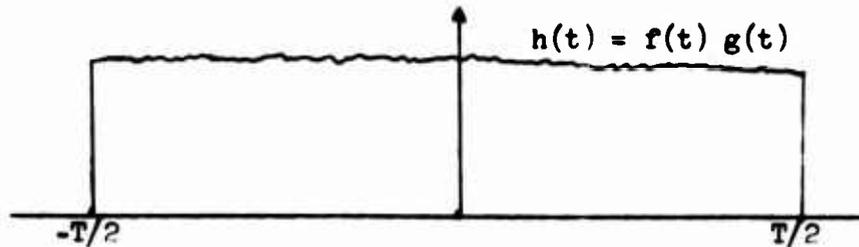


Figure 2

The function $h(t)$ then represents the truncated data set available from which the power spectrum is to be calculated. The power spectrum $P_{ap}(\omega)$ of $h(t)$, representing the apparent power spectrum of $f(t)$, is then

$$\begin{aligned}
 P_{ap}(\omega) &= |\mathfrak{F}(f \cdot g)|^2 \\
 &= |F * G|^2 \\
 &= |F|^2 * |G|^2 \quad , \quad (8)
 \end{aligned}$$

the last step resulting from the fact that g is presumed to be an even function. Thus the true power spectrum

$$P_{true}(\omega) = |F|^2$$

is modified by convolution with $|G|^2$, the Fourier transform squared of the data window. G is called the frequency window by Blackman and Tukey (1958). For the data set shown in Figure A-2, G is the sinc function, shown in Figure 3.

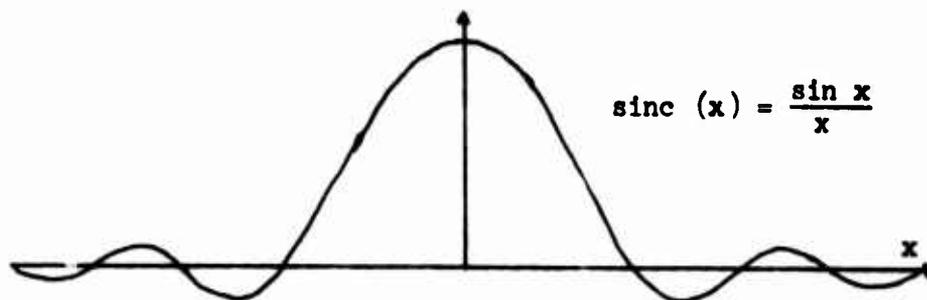


Figure 3

Convolution by the frequency window causes a certain degree of smoothing in the calculated power spectrum and a small amount of leakage via the side lobes from nearby frequency bands into the frequency band of interest. If the computed power spectrum is relatively flat, i.e., has a dynamic range of less than 2 or 3 orders of magnitude, this smearing or leakage causes little or no problem, for the amplitude of the largest (first) side lobe of the sinc function is only on the order of several percent of that of the main lobe. If, however, there are large, well-defined peaks in the power spectrum such large peaks act as a first approximation delta function. When convolved with the frequency window they act to reproduce the window, producing spurious peaks in the power spectrum corresponding to the side lobes of the frequency window. These spurious peaks may be mistakenly identified as structural details of the true power

spectrum when in reality they are merely artifacts created by truncation of the original data set.

B. Reducing Frequency Window Leakage

Because of the frequency window side lobe leakage associated with data function truncation, one is properly concerned with means of reducing or minimizing the undesirable effects of such truncation. Several methods are available for doing this, each depending somewhat on the particulars of how the power spectrum is computed. Three commonly used methods will be described in the following sections, each being intended to illustrate the basic features of and rationale behind each procedure.

1. Data Tapering

One of the obvious methods of reducing the side lobe leakage is to choose the data window $g(t)$ such that its Fourier transform $G(\omega)$ has either no side lobes at all or side lobes that are small compared to the main lobe. Examples of the former are:

$$g(t) = e^{-(|t|/2t_0)^2} \quad (\text{Gaussian})$$

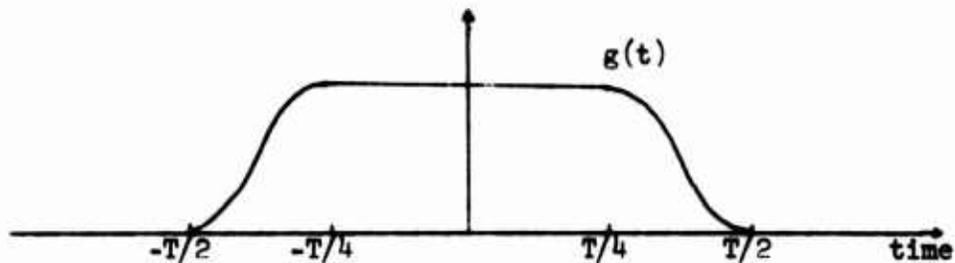
where t_0 is some scale factor. This function has a Fourier transform equal to a Gaussian; and

$$g(t) = \frac{\sin 2\pi \Delta f t}{2\pi \Delta f t} \quad (\text{sinc function})$$

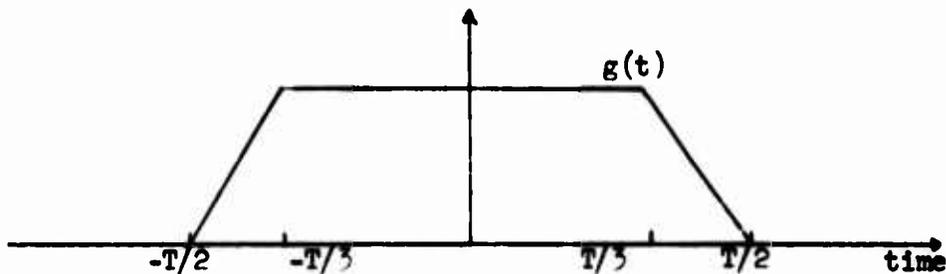
which has a Fourier transform equal to the box-car function.

However, for the side lobes to be eliminated altogether it is necessary to extend these data windows to $\pm \infty$. If they are truncated at some finite value (as they must be in practice), side lobes are again introduced, though they will be smaller than the case where $g(t)$ is the box-car function.

A simpler method is to taper the data set at the ends using data windows indicated in the following sketches:



or



Although side lobes are still present in the frequency windows for each of the above cases, they will be smaller than for the case where the simple box-car data window was used. The smaller side lobes are a result of replacing the abrupt discontinuities of the original box-car data window with more gently sloping functions.

Data tapering is most often performed when the FFT method is used to compute the power spectrum. For a more complete discussion of this topic see Enochson and Otnes (1968).

2. Tapering the Autocorrelation Function

If the MLP method of computing the PSD is used the problem of side lobe leakage is not as simple as it was in the case of computing the PSD directly from its definition. An additional factor for consideration enters when not only the original data set must be truncated, but so also the autocorrelation function. When an MLP calculation is made it becomes advisable, for reasons to be discussed in connection with statistical reliability, to truncate the autocorrelation function at a maximum lag of not more than 10—20% of the length of the data set (Blackman and Tukey, 1958). In order to see what effect this second truncation has, consider the original data set $f(t)$ properly truncated with a data window $g(t)$. The autocorrelation function $\varphi_{11}(\tau)$ then becomes

$$\varphi_{11}(\tau) = [f(t) \cdot g(t)] * [f(t) \cdot g(t)]$$

or

$$\varphi_{11} = (f \cdot g) * (f \cdot g) \quad .$$

Now φ_{11} represents the entire autocorrelation function available after f is truncated by g . To truncate φ_{11} at a lag of 10–20% of the length of the data set therefore involves specifying another function $q(\tau)$, called the lag window, by which φ_{11} is multiplied in order to effect truncation. Let φ'_{11} represent the truncated autocorrelation function. Then

$$\varphi'_{11} = \varphi_{11} \cdot q = [(f \cdot g) * (f \cdot g)] \cdot q \quad .$$

The apparent power spectrum is the Fourier transform of the truncated autocorrelation function so that

$$\begin{aligned} P_{ap}(\omega) &= \mathcal{F}\{[(f \cdot g) * (f \cdot g)] \cdot q\} \\ &= \mathcal{F}\{(f \cdot g) * (f \cdot g)\} * \mathcal{F}(q) \\ &= [\mathcal{F}(f \cdot g) \cdot \mathcal{F}(f \cdot g)] * \mathcal{F}(q) \\ &= [(F * G) \cdot (F * G)] * Q \quad , \end{aligned} \tag{9}$$

where Q (the so-called spectral window) is the Fourier transform of q , the lag window. Now g and q are normally chosen to be even functions, so that

$$\begin{aligned}
 P_{\text{ap}}(\omega) &= (|F|^2 * |G|^2) * Q \\
 &= [P_{\text{true}}(\omega) * |G(\omega)|^2] * Q \quad . \quad (10)
 \end{aligned}$$

We see that, as in section III-A, the true power spectrum has been altered by convolution with $|G(\omega)|^2$, and additionally by convolution with Q . If $q(\tau)$ was the box-car function, then $Q(\omega)$ is the familiar sinc function, not squared. It is this last convolution that can lead to negative values in the apparent power spectrum even though negative values are theoretically impossible in a power spectrum. They are, in this case, merely an artifact due to truncation.

To remove the possibility of negative values for the power spectral estimates, as well as making the side lobes of the window Q smaller, it is once again advisable to tailor the shape of the lag window $q(\tau)$. It is to be tailored in such a way that the side lobes that remain are small in comparison to the main lobe, and damp out quickly with increasing distance from the main lobe. Two lag windows that have been found to do this effectively are:

$$(1) \quad q_1(\tau) = \frac{1}{2} \left(1 + \cos \frac{\pi\tau}{T_m} \right) \quad , \quad -T_m \leq \tau \leq T_m$$

where T_m is the greatest lag used in the autocorrelation function.

The use of this window is called "hanning". A second, more commonly used lag window is

$$(2) \quad q_2(\tau) = 0.54 + 0.46 \cos \frac{\pi\tau}{T_m}, \quad -T_m < \tau \leq T_m .$$

Use of this window is called "hamming".

The two functions q_1 and q_2 , along with their associated transforms Q_1 and Q_2 are shown in Figure 4.

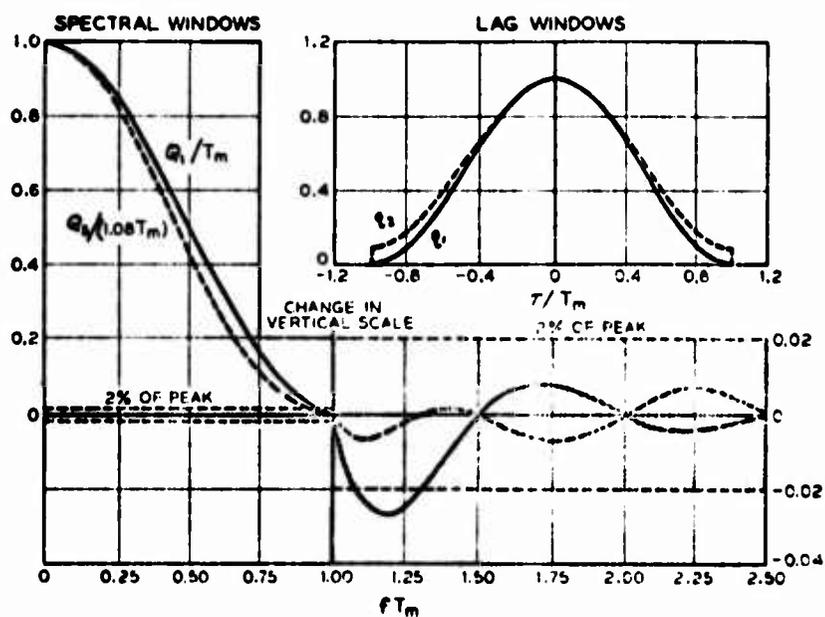


Figure 4

(After Blackman and Tukey, 1958.)

Although in principle $q(\tau)$ would normally be applied to the autocorrelation function prior to transforming, the interchangeability of the integrations associated with the transform and the convolution makes it possible to convolve with $Q(m)$ after the transform has been completed. This has particular advantages when the data are in digital form. In the case of hamming or hanning, the convolution will take the form of a 3-point smoothing formula easily applied to the power spectrum estimates calculated by transforming the autocorrelation function. More will be said about this form of smoothing in section V when a specific power spectrum example is given.

It might be added that when the MLP method for computing PSD's is used it is usually unnecessary to be overly concerned about the effects of the convolution of $|Q(m)|^2$ with $P_{\text{true}}(m)$ [see Eq. (10)]. Since $G(\omega)$ is squared, whereas $Q(\omega)$ is not, the side lobes of $|G(\omega)|^2$ will be unimportant compared to those of $Q(\omega)$. The half-width of the major lobe of $G(\omega)$ is also small (~ 1 order of magnitude smaller) compared to that of $Q(m)$ since the original data set is ~ 10 times longer than $q(\tau)$. Therefore the effects of Q will far outweigh those of G , and it is those effects that hamming or hanning are designed to offset. It is accordingly not necessary to taper the original data set (or pre-whiten; see next section) except in cases of extremely discontinuous spectra, or when extreme care need be taken to assure the validity of the results.

3. Pre-whitening

As was mentioned previously, if there are large, well-defined peaks in the power spectrum such peaks can produce spurious detail in the power spectrum due to frequency or spectral window side lobe leakage. It is for this reason that methods were sought to reduce the side lobes. An alternate method that can be used on occasion is known as "pre-whitening". This procedure involves flattening the power spectrum prior to calculation by passing the data through a filter with a known power transfer function in order to eliminate large peaks and discontinuities. With the peaks and gross discontinuities thus removed, the effective convolution of $|F|^2$ with $|G|^2$ to yield $P_{ap}(m)$ will not act to reproduce the side lobes of $|G|^2$ as would have been the case had the peaks not been removed. Once the power spectrum is computed the inverse of the pre-whitening, the so-called "post-darkening", is applied to the PSD estimates to complete the calculation.

In order for pre-whitening to be used effectively some prior knowledge of the expected shape of the spectrum to be flattened must be available. This is necessary in order to design a filter with the proper power transfer function. An example of how pre-whitening may be used is the following: Suppose we have a data set for which we know approximately the shape of the power spectrum, and suppose it has a very large low (zero) frequency component, as in Figure 5.

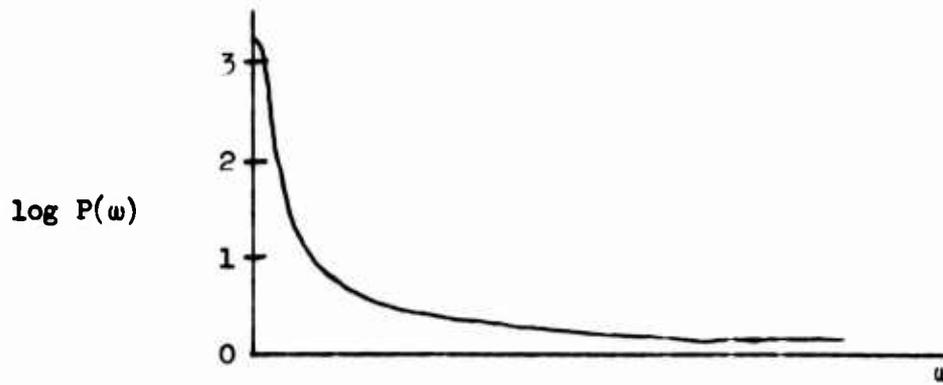


Figure 5

If the power spectrum is computed directly from the data without some measures being taken to compensate for possible side lobe leakage, the apparent power spectrum $P_{ap}(\omega)$ would look something like Figure 6.

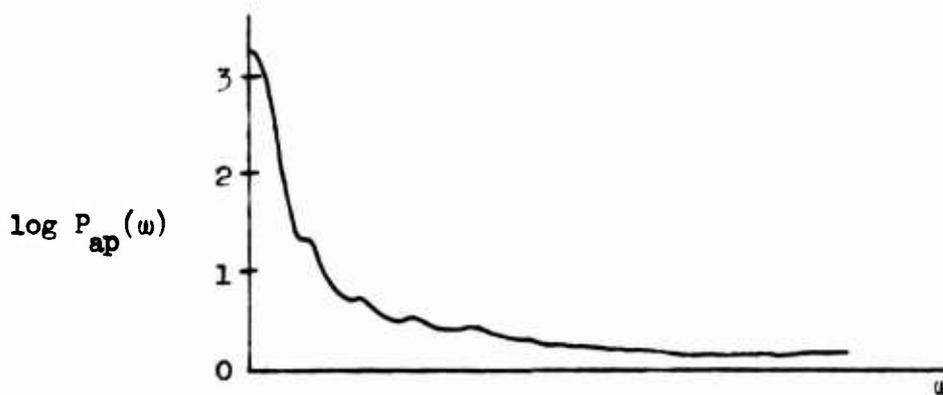


Figure 6

The small scale structure may well be that solely due to side lobe leakage, though in the case where confidence in the results is low this structure can be masked by statistical noise.

Suppose now that the original data $f(t)$ is pre-whitened by convolution with a smoothing function $s(t)$. Then the data set $h(t)$ available from which the PSD calculation is made will be

$$h(t) = f(t) * s(t)$$

or more simply,

$$h = f * s \quad .$$

Then

$$\begin{aligned} P_{ap}(\omega) &= |\mathcal{F}(h)|^2 = |\mathcal{F}(f * s)|^2 \\ &= |F \cdot S|^2 \quad , \end{aligned}$$

or

$$\begin{aligned} P_{ap}(\omega) &= |F|^2 \cdot |S|^2 \\ &= P_{true}(\omega) \cdot |S|^2 \end{aligned} \tag{11}$$

since $s(t)$ is an even function.

Thus, if the original data set is convolved with a smoothing function $s(t)$, the true PSD is modified by the direct product of the square of the transform of $s(t)$. $|S|^2$ is called the power transfer function. To compensate for this at the end of the calculation we multiply by the inverse of $|S(\omega)|^2$ to restore the proper shape to $P(\omega)$.

In the above example suppose we choose a smoothing function

$$s(t) = \begin{cases} \frac{1}{2} \left[1 + \cos \frac{\pi(t - t_0)}{2\Delta\tau} \right] & , \quad |t - t_0| < 2\Delta\tau \\ 0 & , \quad |t - t_0| \geq 2\Delta\tau \end{cases}$$

where $\Delta\tau$ is some scale factor. This smoothing function may be passed over the data as many times as one desires, more smoothing being accomplished with each pass and more of the high frequency components being suppressed.

If the data is in digital form the smoothing function above takes the form such that if $f'(t)$ is the smoothed data,

$$f'_i(t) = \frac{1}{2} f_i(t) + \frac{1}{4} [f_{i-1}(t) + f_{i+1}(t)] \quad . \quad (12)$$

Holloway (1958) showed that for n successive passes of the above elementary filter function through the data, the power transfer function $|S|^2$ becomes

$$|S|^2 = \cos^{2n}(\pi f \Delta t) \quad ,$$

where Δt is the data sample spacing.

The above filter function may be used to effectively remove the low-frequency component in the present example. If the smoothed data (low-pass filtered) is subtracted from the original unsmoothed data, the difference will represent the original data filtered by a high-pass filter with a power transfer function equal to the complement of the original transfer function. Suppose the original data is filtered using this method. The smoothing function applied to the original data set $f(t)$ will have a power transfer function similar to Figure 7.

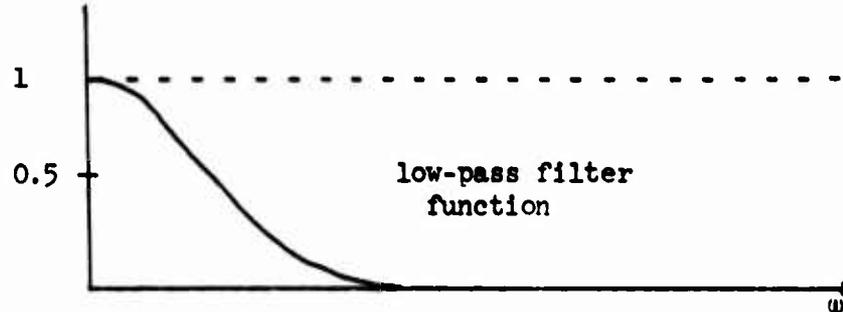


Figure 7

When this smoothed data is subtracted from the original $f(t)$, the resultant power transfer function will be the complement of the function shown above.

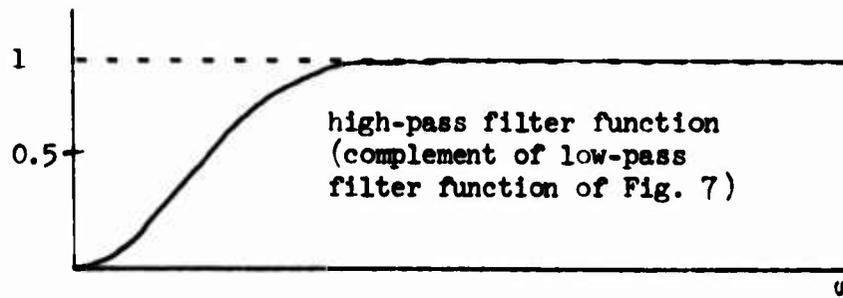


Figure 8

Applied to our example of data with a large low-frequency component, this will effectively flatten the curve to minimize the possibility of side lobe leakage. After the PSD has been computed post-darkening is achieved by multiplying by the inverse of the function shown in Figure 8 to complete the calculation.

For a more complete discussion of the topic of pre-whitening and digital filtering techniques see Blackman and Tukey (1958) and Enochson and Otnes (1968).

IV. DIGITIZED DATA

The discussion of power spectra has been general up to this point, with only an occasional reference to specifics. Since we are here primarily interested in data that appears in discrete, digital form, it is appropriate to specialize to that case. We shall from this point forward consider only the power spectra of data consisting of discrete, equi-spaced samples. The discrete forms of the general equations of section II will be given for both the MLP and FFT calculations. The statistical reliability of PSD estimates will be discussed briefly for each of the two methods, and several considerations helpful for planning will be mentioned. The averaging of several power spectra is also mentioned.

A. Discrete Forms of Relevant Equations

1. MLP Method

The steps required for calculation of a power spectrum using the MLP method may be summarized from the above discussion to be the following:

(1) Pre-whitening. If the power spectrum is known to contain large peaks or discontinuities, the raw data should be pre-whitened by use of appropriate digital filters (high-pass, low-pass, band-pass, or combinations of these). The necessity for this procedure is

somewhat open to interpretation according to one's perception of what constitutes a large peak or discontinuity. My own limited experience over several years is that for a power spectrum with a dynamic range of $> 2-3$ orders of magnitude, pre-whitening to flatten the spectrum prior to its computation is advisable. The example given in section III of a method of constructing a high-pass filter was used successfully by the author (M.S. thesis, 1973). Since, however, the actual method used to pre-whiten will depend on the details of the various power spectra encountered in practice, the reader is referred to chapter 3 of Enochson and Otnes (1968) for a thorough discussion of recursive, non-recursive, and second- and higher-order filters and their application to time series.

(2) Normalizing the Data. Although not mentioned in the previous sections, it is advisable in practice to normalize the data to zero mean and unit standard deviation before calculation of the PSD. Since the calculation of the mean-lagged-products (autocorrelation function) involves the sum of many products, it is easy to terminate a computer calculation of a PSD prematurely due to overflow. Subtracting the mean from the data removes only the zero-frequency cosine term from the PSD, and can be included in the calculation after the remaining following steps are completed. Dividing the (pre-whitened) zero-mean data set by σ reduces the data to unit standard deviation. Correct absolute units can be restored to the final computed PSD if desired by multiplying by σ^2 .

(3) Calculation of the autocorrelation function. If φ_j denotes the j 'th value of the autocorrelation function, the discrete form for the autocorrelation function of the data set $f(t)$ with data sample spacing $\Delta\tau$ containing n discrete values f_i is

$$\varphi_j = \frac{1}{n-j} \sum_{i=0}^{n-j} f_i \cdot f_{i+j} \quad , \quad j = 0, 1, 2, \dots, m \quad , \quad (13)$$

where m is the maximum number of lags in the autocorrelation function. As mentioned in section II, m will generally be limited to 10–20% that of n .

(4) Fourier transform of the autocorrelation function. Since the autocorrelation function is an even function, the discrete form for the Fourier transform becomes the discrete finite cosine series. Applying this to the sequence $\varphi_0, \varphi_1, \dots, \varphi_m$ we obtain as raw estimates for the PSD

$$P_i = \Delta\tau \left[\varphi_0 + 2 \sum_{j=1}^{m-1} \varphi_j \cos \left(ij \frac{\pi}{m} \right) + \varphi_m \cos i\pi \right] \quad , \quad (14)$$

$$i = 0, 1, \dots, m$$

where $\Delta\tau$ is the sample spacing.

(5) Smoothing the raw estimates. The raw estimates calculated in step (4) correspond to Eq. (10)

$$P_{ap}(\omega) = [P_{true}(\omega) * |G(\omega)|^2] * Q ,$$

with a box-car lag window leading to a sinc function spectral window. What remains is convolution with a suitably tailored spectral window Q with small side lobes to complete the calculation. A commonly used window is the hamming window, the digital form of which becomes

$$P_i = 0.54 P_i + 0.23 (P_{i+1} + P_{i-1}) . \quad (15)$$

(6) Post-darkening. If the raw data were pre-whitened in step (1), the last step in the calculation of the PSD will be to restore the true shape of the power spectrum by post-darkening. This process involves multiplying the smoothed estimates of step (5) by the inverse of the pre-whitening filter power transfer function.

The frequency resolution Δf of the resultant spectrum will be

$$\Delta f = \frac{1}{2m \Delta \tau}$$

where

m = the maximum number of lags in the autocorrelation function

and

$\Delta \tau$ = data set sample period.

The maximum frequency of the computed PSD will be

$$f_{\max} = m\Delta f = \frac{1}{2\Delta\tau} \quad (16)$$

in accordance with the sampling theorem.

2. FFT Method

The fast-Fourier-transform technique of computing the PSD of a time series was a major improvement over the MLP method in terms of the actual computer time taken for the calculation. If N is the number of points in a time series, the total computer time needed for an MLP calculation is roughly proportional to N^2 , where for the FFT method it goes approximately as $N(\log N)$. The advantages of utilizing the FFT method whenever many points are being power spectrum analyzed therefore lie on the side of efficiency rather than any fundamental superiority of the method over that of the MLP. As a technique of computing PSD's, it is quickly supplanting the MLP method and is therefore worth studying. An extensive discussion of the FFT computed one-dimensional PSD by Brault and White (1971) provides a thorough introduction to FFT methods and their application to astronomical problems.

Although no attempt will be made here to outline in detail the steps required for FFT calculation of a PSD, the basic steps are as follows:

(1) Pre-whitening. The necessity for pre-whitening the data is less strong when the FFT method is used than it is for the MLP method. The reason for this lies in the fact that the FFT calculated PSD takes the form

$$P_{\text{ap}}(\omega) = P_{\text{true}} * |G(\omega)|^2 ,$$

whereas the MLP method yielded

$$P_{\text{ap}}(\omega) = [P_{\text{true}} * |G(\omega)|^2] * Q(\omega) .$$

The FFT form does not involve a convolution with Q , so that one need only be concerned with the shape of $G(\omega)$. If $g(t)$ is properly specified the side lobes of $|G(\omega)|^2$ can be kept small enough so that very little leakage is present [see step (3) below]. Only in the case where there are exceptionally large peaks or discontinuities in the power spectrum should pre-whitening be necessary. In general, it may be said that in most cases this step will not be necessary at all.

(2) Normalizing the data. It is advisable to normalize the data to zero-mean and unit standard deviation, for the same reasons as given for the MLP method above.

(3) Data window correction. As discussed in section III-A, truncation of a data set can produce spurious detail in the computed PSD. It is therefore necessary to choose a data window $g(t)$ by which

to multiply the time series such that the frequency window $G(\omega)$ will have small side lobes. A window currently in common use is the ten-percent cosine bell, the application of which is called coswinding. For the generalized formula for this data window see Brault and White (1971, Equation 13).

(4) Appending zeros to the data. The most efficient versions of the FFT require the data to consist of a number of points equal to a power of two, although some generalized versions will work with an arbitrary number of points. If a version is used requiring some specific number of points, the original normalized data set to be transformed must have zeros appended to it to bring the total points up to the specified number.

(5) Transforming the data. The normalized data set f_1 is transformed using the forward discrete Fourier series transform to yield Fourier coefficients

$$a_j + ib_j = \frac{\Delta t}{n_0} \sum_{k=0}^{n_0-1} f_k \exp i \left[-jk \frac{\pi}{n_0 - 1} \right], \quad j = 0, 1, \dots, n_0 - 1 \quad (17)$$

where

Δt = data sample spacing.

n_0 = number of data points in the normalized data set, and

$i = \sqrt{-1}$.

(6) Computing the raw spectrum. The raw PSD is just the absolute value squared of the Fourier transform, adjusted to compensate

for the appendage of zeros to the original data set.

$$P_1 = \frac{n_o^2}{n} (a_1^2 + b_1^2) \quad (18)$$

where n = number of points in the original data set.

(7) Smoothing the raw estimates. The raw estimates obtained in step (6), although theoretically correct, may be statistically unreliable. It is possible to increase the statistical reliability by smoothing (convolving) the estimates with a suitable smoothing function. For an excellent discussion on the subject of smoothing raw FFT estimates see Edmonds and Webb (1972).

The frequency resolution (PSD estimate spacing) of the FFT calculated PSD will be

$$\Delta f = \frac{1}{n_o \Delta t} \quad (19)$$

For specifics on the programming of the FFT algorithm, including Fortran indexing peculiarities, one should consult 'Special Issue on FFT and Its Applications to Digital Filtering and Spectral Analysis', IEEE Trans. AU-15, No. 2 (1967). Another special issue on the same topic, IEEE Trans. AU-17, No. 2 (1969), gives an extensive bibliography.

B. The Statistical Reliability of the PSD Estimates

1. Confidence Limits

The calculation of the PSD from a finite number of discrete data points can be expected to have associated with it a set of confidence limits reflecting the presumed statistical nature of the original time series. In theory, if a PSD calculation could be made from an infinite number of data points, one would have absolute confidence in the results. In practice one must settle for a finite number of points from which to make the calculation. Each point in the resultant power spectrum will have a set of "confidence limits" assigned to it reflecting the confidence (in a statistical sense) that the resulting power spectrum is not due solely to randomly distributed data points.

The statistical accuracy of the computed PSD is estimated in terms of "equivalent degrees of freedom", from which the confidence limits are calculated. The degrees of freedom may be thought of as representing the number of estimates of power in the frequency interval Δf , the frequency resolution of the computed PSD. A measure of the probability that an estimate falls within an upper and lower bound, the ratio of which is designated the confidence factor f_c , is given by

$$f_c = 10^{b/(10\sqrt{k-1})} = \exp\left(\frac{2.3 b}{10\sqrt{k-1}}\right) \quad (20)$$

where

f_c = confidence factor for a given confidence,

k = degrees of freedom, and

b = factor depending on the desired confidence, given as follows:

		confidence									
		50%	80%	90%	96%	98%					
b	<table style="border-collapse: collapse; width: 100%;"> <tr> <td style="border-bottom: 1px solid black; padding: 5px 10px;">8</td> <td style="border-bottom: 1px solid black; padding: 5px 10px;">16</td> <td style="border-bottom: 1px solid black; padding: 5px 10px;">20</td> <td style="border-bottom: 1px solid black; padding: 5px 10px;">25</td> <td style="border-bottom: 1px solid black; padding: 5px 10px;">29</td> </tr> </table>	8	16	20	25	29					
8	16	20	25	29							

This is an approximation, but for $k \geq 4$ is very close to more exact calculations based upon chi-square tables (Edmonds, 1966).

The confidence factor f_c may be used as error bars for the computed PSD, being positioned on each data point in such a way that the point falls on the geometric mean of the upper and lower limits of f_c . Another way of stating this is that the upper limit for the confidence limits is equal to the PSD estimate times the square root of f_c ; the lower limit equals the estimate divided by the square root of f_c . If the PSD is plotted on a semi-log scale the confidence limits will be centered on each point.

A plot of f_c as a function of degrees of freedom k for several different confidences is shown in Figure 9. The ordinate expresses f_c in Db; to determine f_c one goes across to the straight line labeled "factor", then reads f_c off the abscissa. As an example, for $k = 30$

the 90% confidence factor expressed in D_b is seen to be ≈ 3.8 , for which $f_c \approx 2.7$.

The next two sections will consider formulas for determining k for each of the two methods of computing PSDs.

2. k for the MLP Calculation

The number of degrees of freedom k for the one-dimensional MLP calculated PSD is given by (Blackman and Tukey, 1958)

$$k = 2 \left(\frac{N}{M} - \frac{1}{3} \right)$$

where

N = the number of data points in the data set, and

M = the maximum number of lags in the autocorrelation function
 = the number of points in the computed PSD.

As can be seen from this formula, k is nearly proportional to the ratio N/M . In order to achieve maximum confidence in the PSD estimates it is necessary that k be made as large as possible; this will insure that the confidence factor f_c [Eq. (20)] will be small. N is usually some fixed number of points, so M is therefore chosen to be small relative to N . It is for this reason that M is normally chosen to be not more than 10–20% of N .

3. k for the FFT Calculation

The number of degrees of freedom k for the one-dimensional FFT calculated PSD is given by (Tukey, 1967)

$$k = 2p \left(\frac{N - N_T}{N_0} \right)$$

where

N = the number of points in the original data set,

N_T = the number of points tapered by the data window $g(t)$,

N_0 = the total number of data points after zeros have been appended, and

p = the effective number of points involved in smoothing of the raw PSD estimates.

Although the MLP and FFT formulas for k appear to be superficially different, it is not difficult to show that the confidence limits calculated from a given k are essentially equivalent for the two cases, as would be expected.

C. Planning Considerations

In the previous sections the basis of a PSD calculation was discussed with appropriate equations given. In a practical application some thought must be given to the problem of choosing data sample spacing, frequency resolution, and the frequency range over which the power spectrum is to be calculated. This section will deal only with

considerations to be made in performing an MLP calculation; similar considerations will apply to an FFT calculation.

1. Choosing $\Delta\tau$ and f_{\max}

The raw data from which the PSD is to be calculated is assumed to consist of discrete, equi-spaced samples of period $\Delta\tau$. Then if f_{\max} denotes the maximum frequency for which PSD estimates are obtained we have from the sampling theorem

$$f_{\max} = \frac{1}{2\Delta\tau} .$$

f_{\max} is clearly independent of the total number of data points and the maximum lag M of the autocorrelation function. It depends solely on the sample spacing. If in an analysis one wishes to examine the PSD up through a specific frequency, this formula shows what the corresponding minimum sampling frequency must be. Likewise, if it is desired only to compute the PSD for a limited frequency range, by choosing the correct $\Delta\tau$ the resulting PSD will have a frequency range of exactly the right size. This fact is helpful in minimizing the number of data points required in a calculation. For example, if one were interested in examining the PSD of a set of data only in the frequency range 0—5 Hz, the sampling period $\Delta\tau$ would be 0.1 sec. Sampling more often than this would increase f_{\max} beyond the range of interest, increase the total number of data points, and thus the machine calculation time, and generally would not add any information.

If the sampled data already exists for which the power spectrum is to be calculated, it is possible to adjust $\Delta\tau$ to near the desired value by (a) decimation, using only every p'th point of the original data or (b) averaging, averaging by groups of p points. The former method increases $\Delta\tau$ by a factor of p and maintains the standard deviation (for random or near-random data) about the mean. The latter increases $\Delta\tau$ by a factor of p but decreases the standard deviation about the mean by a factor of \sqrt{p} . For further discussion on these methods consult Enochson and Otnes (1968).

2. Choosing M and Δf

The frequency resolution Δf of the calculated PSD is

$$\Delta f = \frac{1}{2M}$$

where M is the maximum lag in the autocorrelation function. This formula may be used for either determining in advance of a calculation what the frequency resolution will be, or for determining M for a given desired Δf . As discussed in section B, M should be small relative to the total amount of data. This fact must also be taken into account when planning a PSD calculation.

As an example of how the foregoing considerations may be used, suppose we wish to calculate the PSD of a data set for the frequency

range 0—5 Hz. Suppose further that we wish the frequency resolution Δf to be 0.2 Hz, providing a total of 26 points (including the end-points) in the power spectrum, and that the 90% confidence factor is to be < 2.0 . Then

$$\Delta\tau = \frac{1}{2(5)} = 0.1 \text{ sec} \quad .$$

$$M = \frac{1}{2(0.2)} = 2.5 \text{ sec}$$

= the maximum lag of 26 data points.

From Figure 9 we find that for the desired confidence we must have $k \geq 45$, from which

$$T \geq \frac{Mk}{2} = \frac{2.5(45)}{2} = 61 \text{ sec}$$

for which

$$N = 610 \text{ data points.}$$

As a second example suppose a data set already exists consisting of 500 points with sample spacing 1 sec. If the autocorrelation function is truncated at 10% the length of the data set, we calculate f_{\max} , Δf , k , and f_c (90%) to be:

$$f_{\max} = \frac{1}{2\Delta\tau} = 0.5 \text{ Hz} \quad ,$$

$$\Delta f = \frac{1}{2M} = \frac{1}{2(50)} = 0.01 \text{ Hz} \quad .$$

$$k = 2 \left(\frac{N}{M} - \frac{1}{2} \right) = 2 \left(\frac{500}{50} - \frac{1}{2} \right) = 19.7 \quad , \text{ and}$$

$$f_c (90\%) = 2.9 \quad .$$

From the above simple examples it is seen that M , N , $\Delta\tau$, f_c , Δf , and f_{\max} are to a degree interrelated. Therefore one must be somewhat judicious in their specification in order to achieve the maximum amount of usable information in a PSD calculation. For example, one can achieve a very high degree of statistical reliability by making M very small. However this would be at the expense of the frequency resolution. In general, for a given data set there is a trade-off between statistical reliability and frequency resolution. This problem can be surmounted by simply increasing N (using more data) but then the computing time increases, and so on.

D. Averaging Power Spectra

It is occasionally desired to study the average characteristics of power spectra over long periods of time. Although it is possible to compute an average power spectrum over a long data set, it is

sometimes more efficient to break it up into shorter sets, compute the PSD for each individual data set, then average the results. This procedure is also necessary if, for example, several short, non-contiguous data sets of varying lengths exist for which one wishes to extract an average power spectrum. The validity of the averaged results will depend on the stationarity of the data; for data which is non-stationary the results will be influenced by the lengths and number of data sets used in the calculation. [For a short discussion on this point see Sentman (1973).] The following sections apply to MLP calculated PSD's, though similar considerations would apply to FFT calculated PSD's.

1. Averaged Power Spectra from Data Sets of Equal Lengths

If it is assumed that the frequency resolution Δf is identical for each PSD comprising the average, the statistical reliability of each is the same. Then

$$\bar{P}_1 = \frac{1}{N} \sum_{j=1}^N \sigma_j^2 P_{1j}$$

where

\bar{P}_1 = i'th point in the averaged power spectrum,

P_{1j} = i'th point in the j'th power spectrum,

N = the number of spectra being averaged, and

σ_j = standard deviation about the mean of data in the original j'th (pre-whitened) data set. If the data in the j'th data set were divided by σ_j after the mean was removed prior to calculation of the power spectrum, this weight is necessary to restore the proper relative units to P_{1j} . If the data were not normalized this weight is equal to one.

2. Averaged Power Spectra from Data Sets of Different Lengths

If the individual spectra comprising the average are computed from data sets of different lengths, the statistical reliability of each PSD is different. If Δf is identical for each individual PSD, the expression for averaging becomes

$$\bar{P}_1 = \frac{1}{N} \sum_{j=1}^N \sigma_j^2 \exp \left[\frac{-2.3 b}{20\sqrt{k_j} - 1} \right] P_{1j}$$

where

k_j = degrees of freedom in the j'th computed power spectrum,

and

$b = 8$, for 50% confidence limits.

The exponential weighting factor must be included to properly weigh individual spectra according to its probable error. The uncertainty in the spectra is taken to be the probable error, or the square root of the 50% confidence factor defined in Eq. (20).

Statistical Reliability of Averaged Spectra

Confidence limits for the averaged spectrum are computed by assuming that its equivalent degrees of freedom \bar{k} equal the sum of the degrees of freedom in the individual spectra comprising the average.

$$\bar{k} = \sum_{j=1}^N k_j \quad .$$

It can easily be shown that if the statistical "noise" present in each of the individual spectra is treated as a random fluctuation about the true power spectrum, the above expression for calculating \bar{k} results in confidence limits that shrink at exactly the same rate as the "noise" when more and more spectra are averaged.

V. AN EXAMPLE OF A POWER SPECTRUM CALCULATION

As an example of how the information contained in the previous sections may be applied, the following will serve to illustrate the basic features of an MLP calculated power spectrum. The example given is from a calculation made in conjunction with the study of oscillatory phenomena in the solar atmosphere (Sentman, 1973).

The raw data consisted of antenna temperature 5 sec data samples of solar microwave emission recorded on the North Liberty Radio Observatory 2-cm radiometer. Individual data sets ranged in length from 4—12 h. The power spectrum of each data set was to be calculated, and the average of all the individual spectra computed to obtain an average power spectrum for all the data sets.

The frequency range of interest to this study was 0—15 mHz ($1 \text{ mHz} = 10^{-3} \text{ Hz}$), or $f_{\text{max}} = 15 \text{ mHz}$. A sampling time $\Delta\tau$ of $1/2(15 \times 10^{-3}) = 33.3 \text{ sec}$ was thus indicated. The nearest that one could come to this figure using 5 sec data samples was either 30 sec or 35 sec, corresponding to averaging the 5 sec samples by groups of 6 or 7, respectively. Averaging by groups of 6 was chosen, yielding an effective sampling time $\Delta\tau = 30 \text{ sec}$ and a maximum frequency $f_{\text{max}} = 16.7 \text{ mHz}$. A typical data set with 30 sec resolution (effective sampling time) is shown in Figure 10.

It was known in advance of the calculation (by trial runs on several data sets) that the power spectra all contained a very large peak at near zero frequencies, thus indicating a need for pre-whitening. High-pass smoothing was achieved by means of the method described in section III-B by making 10 passes through the data with the smoothing function described by Eq. (12). The resulting low- and high-pass power transfer functions are shown in Figure 11. A maximum lag of 25 min (= 50 lags \times 30 sec) was chosen to balance frequency resolution against statistical reliability. This resulted in a frequency resolution $\Delta f = 0.33$ mHz. The degrees of freedom k therefore ranged from 18.5 (4 h data set) to 56.9 (12 h data set), providing the high degree of statistical reliability necessary for the study (very low amplitude fluctuations were being sought).

The data normalization and power spectra calculations were achieved using the subroutine listed in Appendix I. After the power spectrum was calculated it was post-darkened to compensate for the pre-whitening by multiplying with the inverse of the high-pass power transfer function shown in Figure 11. An example of the resulting spectra with confidence limits, normalized to a value of 10 in the range of 4–5 mHz for display purposes, is shown in Figure 12 for the frequency range 0–15 mHz. All calculations were carried out on a Univac 418 computer.

FIGURE CAPTIONS

- Figure 9 The confidence factor as a function of degrees of freedom k (see page 35).
- Figure 10 Typical plot of antenna temperature versus time with 30 sec time resolution. Data records used to compute power spectra were chosen to exclude the end pieces of each data day.
- Figure 11 Low-pass and high-pass filter functions $R(f)$ and $R'(f)$ used to pre-whiten the data prior to calculation of the power spectra. Post-darkening is achieved by multiplying the resultant spectra by $1/R'(f)$.
- Figure 12 Power spectrum of the single record containing a statistically significant peak near 4 MHz.

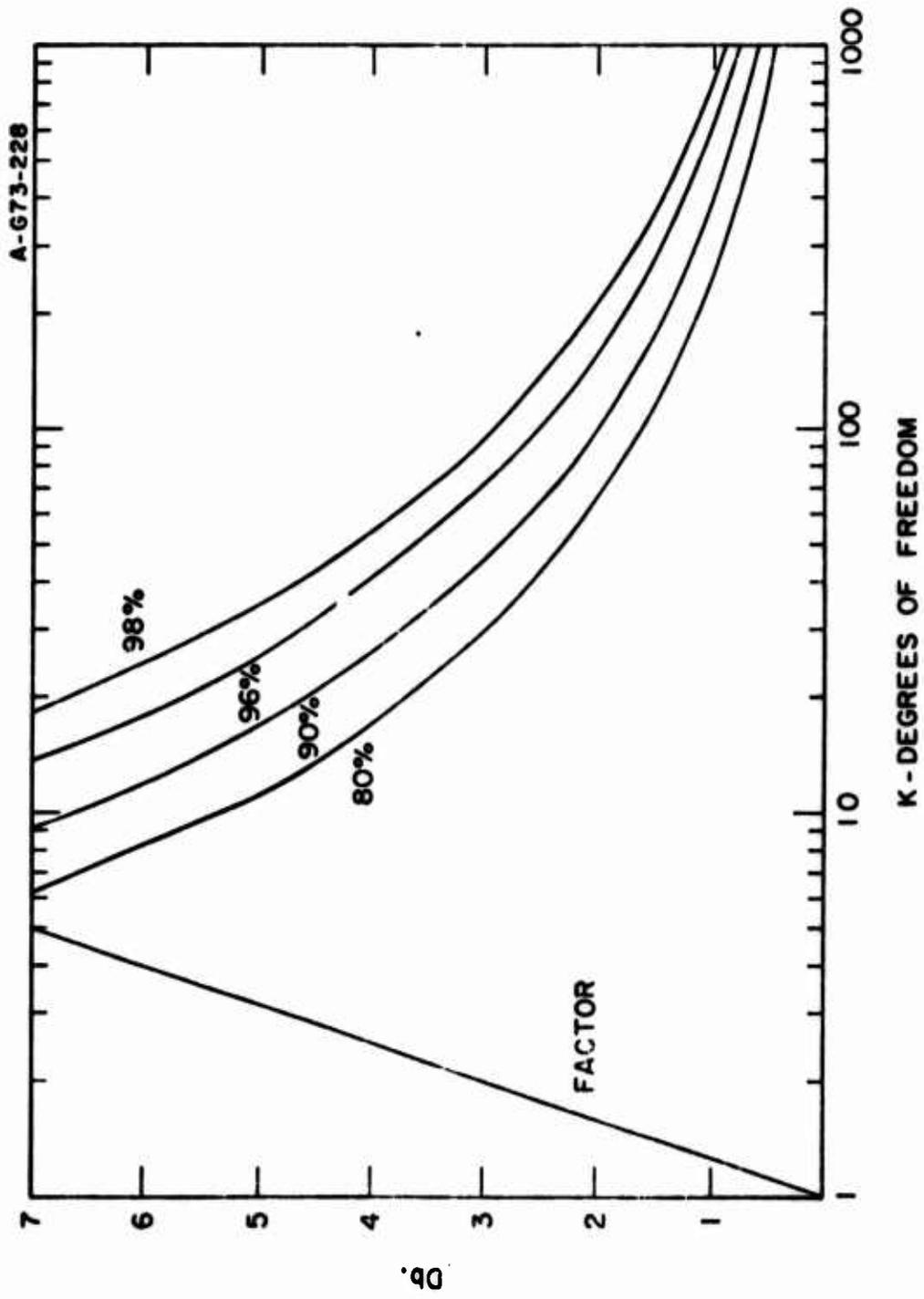


Figure 9

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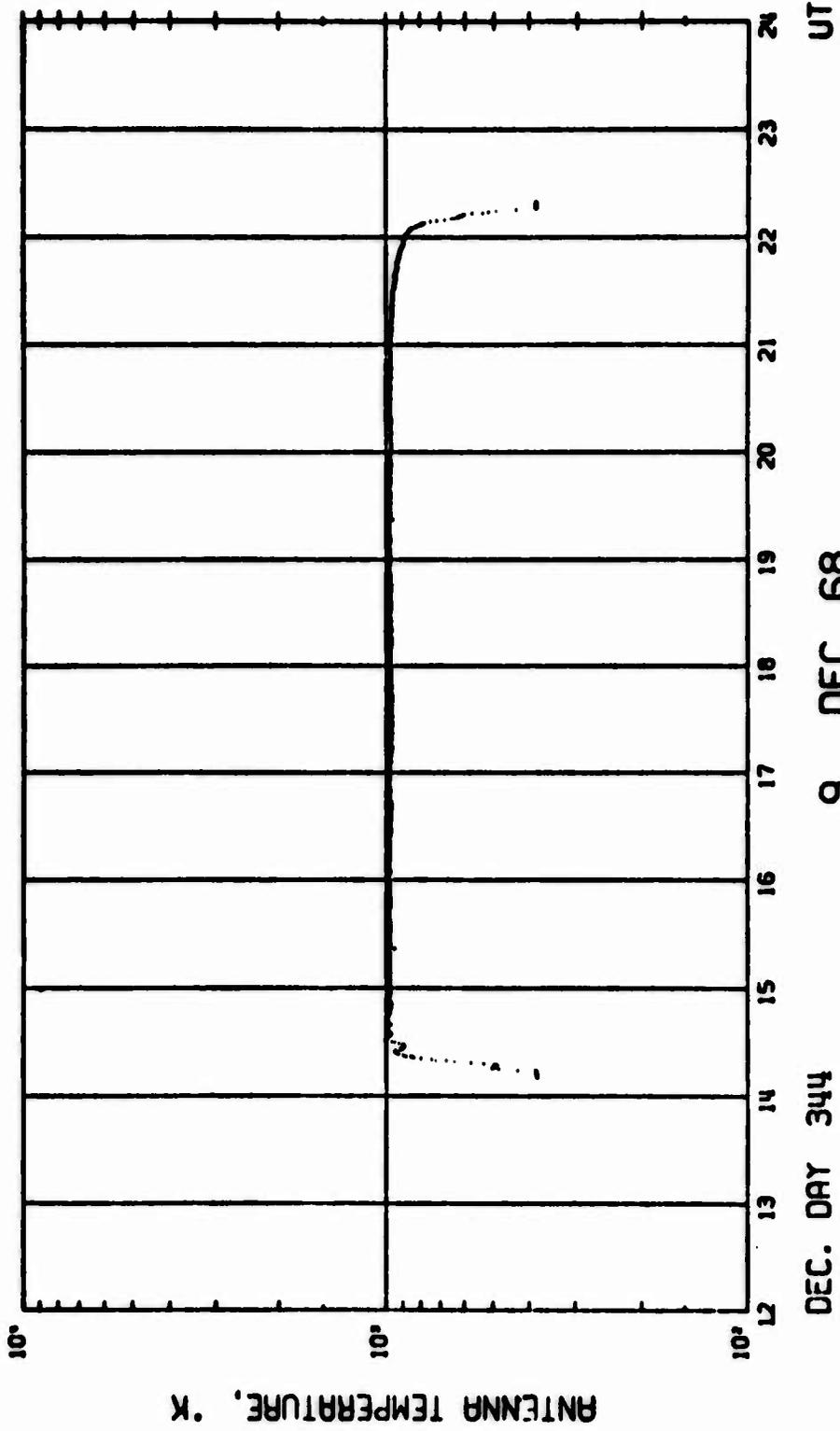


Figure 10

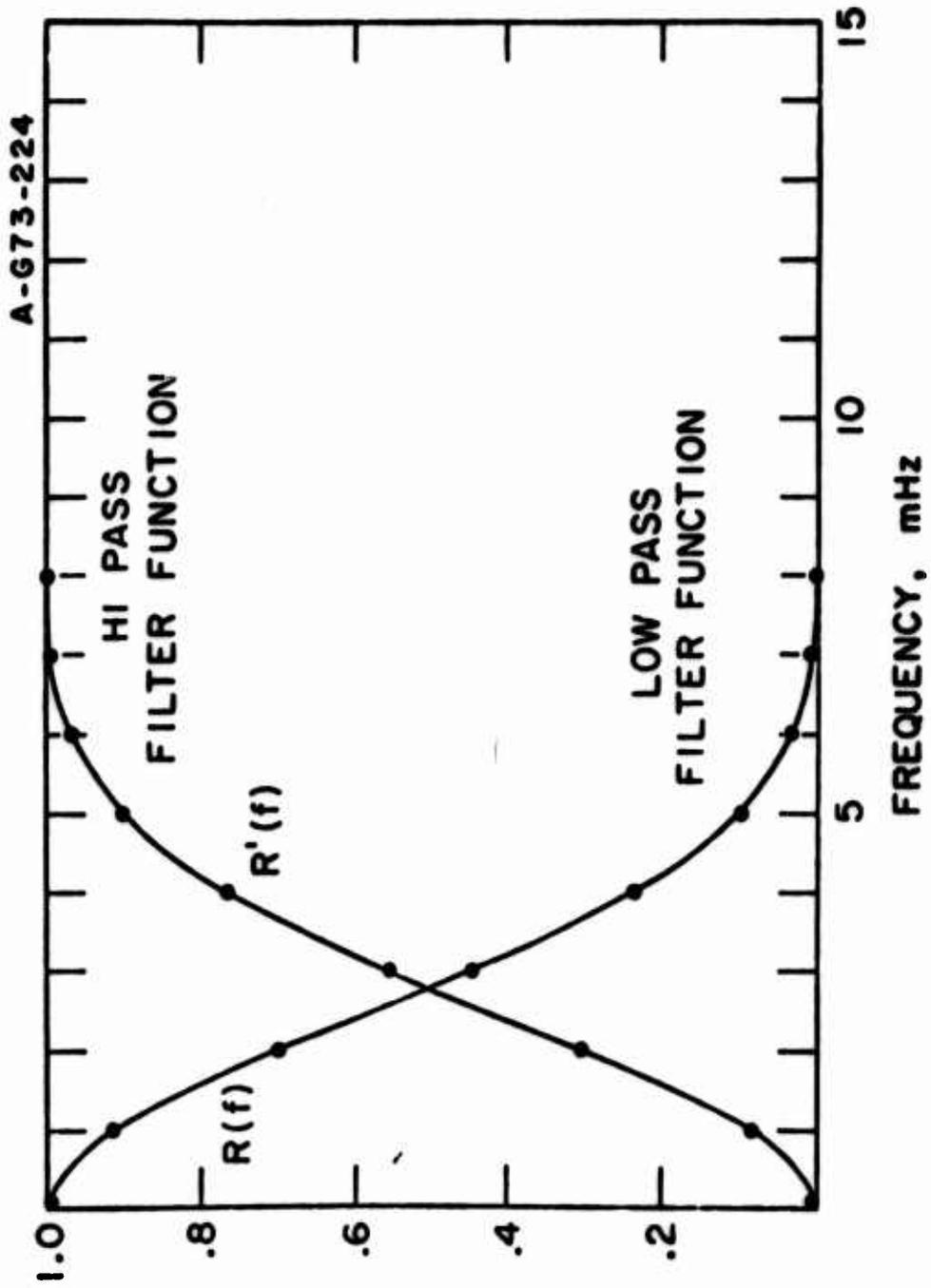


Figure 11

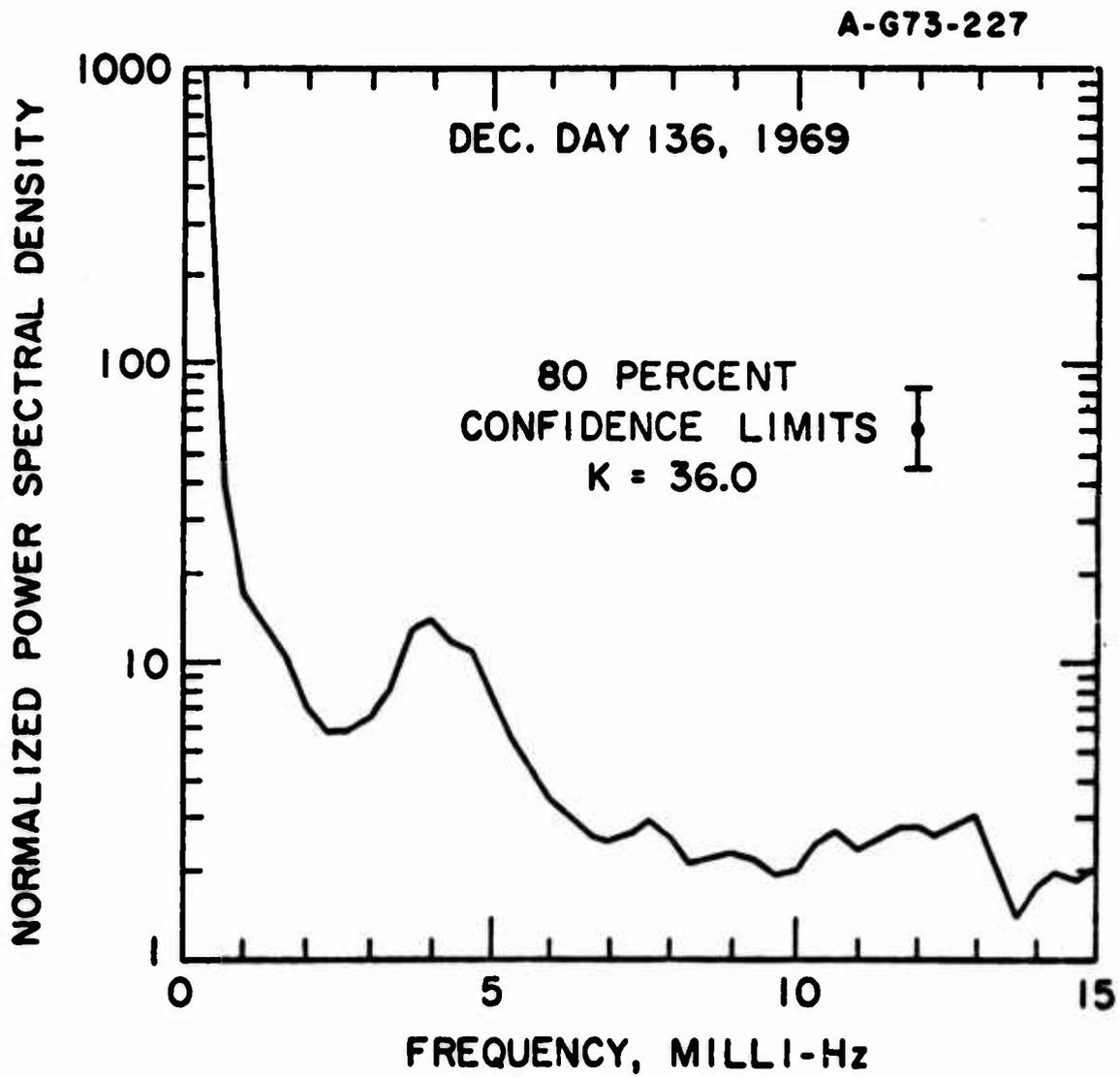


Figure 12

APPENDIX I

A FORTRAN SUBROUTINE FOR CALCULATING POWER SPECTRA

The following is an example of a subroutine for an MLP calculation of a power spectrum. Pre-whitening is assumed to have been completed prior to entry into the subroutine, and post-darkening and conversion to absolute units from normalized units is assumed to take place after return.

The program was written from the definitions for the autocorrelation function and discrete cosine transform. However, to facilitate the transform operation a cosine table is constructed and a table look-up procedure is incorporated into the program rather than requiring a double precision cosine to be computed each time it is needed. The table is constructed in the first call of the subroutine and each time the autocorrelation function maximum lag is changed; succeeding calls use the table already constructed.

As shown below, the program will accommodate a maximum of 1500 data points with an autocorrelation function maximum lag of 500. These figures may be raised or lowered as desired by dimensioning the relevant arrays accordingly.

A. Subroutine Arguments**Input variables:**

- X - Double precision array containing data to be power spectrum analyzed
- N - Integer specifying the number of data points in X (may be smaller than the dimension size of X)
- MA - Integer specifying the maximum number of lags for the autocorrelation function (may be smaller than the dimension size of R)

Output variables:

- U - Single precision array containing $M + 1$ hamming smoothed normalized power spectral estimates
- R - Double precision array containing $M + 1$ values of the normalized autocorrelation coefficients
- XBAR - Double precision variable for the mean of the input data set
- SX - Double precision variable for the standard deviation of the input data set. This variable is necessary if absolute units are to be calculated for the power spectrum (not done here)

B. Subroutine

```

SUBROUTINE SPECTR(X,N,MA,U,R,XBAR,SX)
DOUBLE PRECISION X,AL,CS,XBAR,SX,R
DOUBLE PRECISION FAC,ARG,DCOS,DBLE,DSQRT,PI,AEND
DIMENSION X(1500),U(501),R(501),CS(501),AL(501)
DATA PI/.3141592654D+01/,M/O/

C
C      NORMALIZE DATA TO ZERO MEAN AND UNIT STANDARD DEVIATION
XBAR=0.0
DO 3 I=1,N
3 XBAR=XBAR+X(I)
XBAR=XBAR/DBLE(FLOAT(N))
SX=0.0D+00
DO 6 I=1,N
X(I)=X(I)-XBAR
6 SX=SX+X(I)*X(I)
SX=DSQRT(SX/DBLE(FLOAT(N)))
DO 7 I=1,N
7 X(I)=X(I)/SX

C
C      BUILD COSINE TABLE .CS. FOR INTERVAL .0. to .PI.
IF(MA.EQ.M) GO TO 200
M=MA
MP=M+1
AVERG=DBLE(FLOAT(M))
DO 2 I=1,MP
ARG=DBLE(FLOAT(I-1))
ARG=(PI*ARG)/AVERG
2 CS(I)=DCOS(ARG)
200 CONTINUE

C
C      CALCULATE AUTOCORRELATION COEFFICIENTS
DO 30 J=1,MP
R(J)=0.0D+00
JP=J-1
IEND=N-JP
AEND=DBLE(FLOAT(IEND))
DO 25 I=1,IEND
INDX=I+JP
25 R(J)=R(J)+X(I)*X(INDX)
30 R(J)=R(J)/AEND
C

```

C CALCULATE POWER SPECTRUM
C (FOURIER TRANSFORM A/C FUNCTION .R.)

MX2=M*2
MPX2=MX2+2
MM=M-1
DO 40 J=1,MP
AL(J)=0.0D+00
JP=J-1
DO 35 K=1,MM

C
C CALCULATE INDEX .INDCS. FOR RETRIEVING
C PROPER COSINE FROM TABLE

INDCS=MOD((JP*K),MX2)+1
IF(INDCS.GT.MP) INDCS=MPX2-INDCS
35 AL(J)=AL(J)+2.0D+00*R(K+1)*CS(INDCS)
FAC=1.0D+00
IF(MOD(JP,2).EQ.1) FAC=-1.0D+00
40 AL(J)=AL(J)+R(1)+R(MP)*FAC

C
C APPLY HANNING SMOOTHING FUNCTION TO ESTIMATES .AL.
C TO YIELD SMOOTHED POWER SPECTRUM ESTIMATES .U.

U(1)=SNGL(0.54D+00*AL(1)+0.46D+00*AL(2))
U(MP)=SNGL(0.54D+00*AL(MP)+0.46D+00*AL(M))
DO 50 I=2,M
50 U(I)=SNGL(0.54D+00*AL(I)+0.23D+00*(AL(I-1)+AL(I+1)))
RETURN
END

LIST OF REFERENCES

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