Modern Techniques of Power Spectrum Estimation

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Abstract—**The paper discusses the impact of the fast Fourier transform on the spectrum of time series analysis. It is shown that the computationally fastest way to calculate mean lagged products is to begin by calculating all Fourier coefficients with a fast Fourier transform and then to fast-Fourier-retransform a sequence made up of $a_k^2+b_k^2$ (where a_k+ib_k are the complex Fourier coefficients). Also discussed are raw and modified Fourier periodograms, bandwidth versus stability aspects, and aims and computational approaches to complex demodulation. Appendixes include a glossary, a review of complex demodulation without fast Fourier transform, and a short explanation of the fast Fourier transform.**

I. The Overall Situation

THE PRACTICE of spectrum analysis is entering either its third or fourth era. The periodogram came, proved unsatisfactory, and left. The estimation of spectra via mean lagged products came, helped us to learn many things about the essential limitations of the problem, and proved effective in answering many questions. Complex demodulation was well on its way, once disk memories had changed the balance of computational effort, toward a replacement of the mean-lagged-products route, both because of its savings in computational effort and because it provided simpler and more effective approaches to less obvious questions, such as those related to lack of stationarity. Today the fast Fourier transform has upset almost all our computational habits, and has greatly reduced computational effort.

The theory that is supposed to underlie the practice of spectrum analysis is at least approaching a major transition of its own. In Schuster's day, it would seem, we thought of a single function and its decomposition. Through the decades, probabilistic models, initially often based upon stationary Gaussian distributions, played their parts. (Only recently have we begun to use nonstationary and nonGaussian models to guide our analysis.) Some time series, like earthquakes, are "signals" in the sense that a "repetition" would be an exact copy, while others, like ocean waves from a distant storm, are "noise" in the sense that a "repetition" would have only statistical characteristics in common with the original. The time is now ripe to study our procedures from both points of view: How will they behave when applied to signals? How will they behave when applied to noise? At present, however, this development has not been carried far enough for us to be able to go usefully beyond a general indication of things to come.

Spectrum analysis can mean many different things. The cross-spectrum has long taught us more than has the spectrum, both in two-series problems and in many-series problems. Today, the bispectrum [1], [2], the cepstrum and pseudo-autocorrelations [3], and the study of complex demodulates [4], [2] are all contributing to our knowledge. Fortunately, the impact of modern techniques upon all of these approaches has been rather similar. Thus, we can illustrate much of general application by concentrating on the simple spectrum and complex demodulates.

II. Real and Complex Fourier Analysis

Given a real function of time, expansions in terms of cos ωt and sin ωt with real coefficients, and expansions in terms of $e^{+i\omega t}$ and $e^{-i\omega t}$ with complex conjugate coefficients are trivially equivalent. Both in ease of computation, and, especially, in suggestiveness of computational approaches there are, however, real though minor differences. In this paper, we shall be discussing the subject in terms of the complex expansions, which seem to have the edge.

III. The Fast Fourier Transform

We are used to thinking of the successive values of a time series written out in a long line. We can also write them out (from left to right) in the successive lines (ordered from top to bottom) of a rectangular table. When the number of columns is a divisor of the number of values the result is a rectangular array.

If we want to make a Fourier transform of our rc points (where there are r rows and c columns) by finding the rc coefficients of a (finite) Fourier series that will exactly reproduce the rc given values, it is true, though not obvious, that we can begin by doing c parallel Fourier transforms, each of length r, on the individual columns, and then combine the results thus obtained. This "factoring" saves arithmetic, and if repeated many times, saves much more arithmetic. (For more detail see Appendix III.)

In the particular case of two columns, where we wish to extend a Fourier series corresponding to the r elements in the first column to a Fourier series with twice as many coefficients corresponding to all $2r$ elements

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in both columns, the existence of this possibility was pointed out by Danielson and Lanczos [5] in a paper recently brought to light by Rudnick [6]. The general case was pointed out by Good [7], and taken seriously by Cooley and Tukey [8] who stressed the advantages of factoring into many small factors.

If we have $N=2^n$ values, we require about $2nN = 2N\cdot\log_2 N$ operations to evaluate all N corresponding Fourier coefficients. In comparison with the number, a large fraction of N^2, required by conventional procedures, this number is so small as to completely change the computationally economical approach to various problems. For $N=8192$ points, and an IBM 7094 computer, Cooley reports about 8 seconds for the evaluation of all 8192 Fourier coefficients. Conventional procedures take on the order of half an hour.

IV. The Paradox

One reason for the rise of the mean-lagged-product approach to spectrum analysis was computational economy. It took markedly fewer operations to calculate perhaps a tenth as many mean lagged products as there were data points, and then to Fourier transform the results, than it did to calculate all the Fourier coefficients. [The dream of calculating all these coefficients lurked offstage, however, and led Simpson, for example, to develop a procedure based upon progressive (binary) digiting for calculating all the Fourier coefficients when the data values had, or could be treated as having, limited accuracy.] We all "knew" that the efficient route was via mean lagged products.

As Sande [9] has shown, the fast Fourier transform has changed all this. The computationally fastest way to calculate mean lagged products is to begin by calculating all Fourier coefficients (of an extended series) with a fast Fourier transform and then to fast-Fourier-retransform a sequence made up of $a_k^2+b_k^2$ (where a_k+ib_k are the complex Fourier coefficients). The key device is to border the data values with enough zeroes to make the required noncircular sums of lagged products equal to the corresponding circular sums of lagged products, which arise directly from the Fourier retransformation. If one wants, for example, the first 500 mean lagged products based on $3596(=4096-500)$, the computing time is cut by a factor of 12. Thus, the efficient route now goes via Fourier coefficients to the mean lagged products.

This possibility arises because mean lagged products are essentially the elements in the convolution of two series, one the original data, and the other the original data turned end for end. (The close relation of convolution to the Fourier transform has long been an important commonplace of real analysis.) As a result of the rise of the fast Fourier transform, whether or not one goes through mean lagged products has become a computational detail.

Sande, Stockham, and Helms are among those who recognized the generality of the gain in calculating convolutions via the fast Fourier transform. Stockham [10], in particular, has made it clear how to take advantage of the fact that one of the sequences to be convolved is shorter than the other. With present techniques a conservative estimate of the break-even point puts it at about 25 for the length of the shorter series [11].

V. Raw and Modified Fourier Periodograms

How then shall we estimate the spectrum? The first step is to calculate all the Fourier coefficients a_k+ib_k. Once it would have been "obvious" that the next step would be to calculate the entries $a_k^2+b_k^2$ that make up the raw Fourier periodogram. Today we are more concerned with the nature of the "windows" corresponding to the a_k, the b_k, and the $a_k^2+b_k^2$.

The finite Fourier transform is perfect for the frequencies $\omega_0, \omega_1, \cdots, \omega_k, \cdots$, corresponding to the Fourier coefficients actually calculated. Specifically, if we add $C_j \cos(\omega_j t+\phi_j)$ to the value for time t, doing this for all values to be transformed, we will alter the values of a_j and b_j, but leave wholly untouched (except for roundoff error) those of the other a_k and b_k. If we add $C\cos(\omega t+\phi)$, where ω is none of the ω_j, then every a_j and b_j will be affected, the effects having alternating signs and decaying slowly (like $1/|\omega-\omega_k|$) as ω_k recedes from ω. So slow a decay—so much leakage—is often unacceptable.

The simplest approach is to hann the Fourier coefficients, either directly or by the use of a data window before Fourier transformation. It is important to correct for leakage before squaring and adding; linear modification is desirable; quadratic modification, as by convolving neighboring $a_k^2+b_k^2$ with apparently suitable coefficients, is nearly useless as a means of reducing leakage.

If we consider the hanned Fourier coefficients

$$A_k = -(1/4)a_{k-1} + (1/2)a_k - (1/4)a_{k+1}$$

and

$$B_k = -(1/4)b_{k-1} + (1/2)b_k - (1/4)b_{k+1}$$

(where the $-$ signs would be replaced by $+$ signs, both here and in related formulas following, if we were to center our values of t at 0), we find that their windows fall off, not like $|\omega-\omega_k|^{-1}$ but like $|\omega-\omega_k|^{-3}$, greatly reducing problems with leakage. Accordingly, $A_k^2+B_k^2$ may prove a satisfactory replacement for $a_k^2+b_k^2$. (Under some circumstances it is; under others, we can do still better.)

Notice that we have convolved $-\frac{1}{4}$, $\frac{1}{2}$, and $-\frac{1}{4}$ with the Fourier coefficients. Alternatively, we could have reached the same end by multiplying the data values X_t by a suitable function of time. If t runs from 0 to $T-1$, this function turns out to be

$$\frac{1}{2}\left(1 - \cos 2\pi\frac{t}{T}\right)$$

which is exactly a cosine bell.

To modify the periodogram by linear hanning can be done equally well in two ways: 1) convolving $-\frac{1}{4}$, $\frac{1}{2}$, and $-\frac{1}{4}$ with the Fourier coefficients or 2) multiplying a cosine bell into the input data. (The choice is only a computational one.) There will be similar choices for any of the other simple modifications of the periodogram that we choose to consider.

Whatever modification we choose, each $A_k^2+B_k^2$ will follow a simple exponential distribution when the original observations are a sample from a Gaussian process, and can thus provide only 2 degrees of freedom. Spectrum estimates of useful stability will require adding together several or many such sums (for adjacent frequencies). It is for their contributions to such sums that we calculate either raw or modified periodograms.

VI. Balancing Bandwidth and Stability

The need to balance bandwidth of a spectrum estimate, which it is natural to make narrow, against the estimate's statistical stability, which it is natural to make great, is by now almost commonplace. In dealing with noise-like data this can be the remaining decision of crucial importance, provided we are otherwise using good techniques.

One difference between noise-like data and certain kinds of signal-like data is now apparent. Suppose that our input is signal-like, and is essentially the result of differential attenuation of the frequencies of an initial signal that differed from zero for only a very short duration (as compared to the spacing between our observations). Under these conditions, both phases and amplitudes will usually be reasonably smooth functions of frequency. Unless measurement or background noise is of major importance, our main concern is that the quantities we assess are really appropriate to their nominal frequencies. Statistical stability of the estimates will then be a minor consideration. Accordingly, our main aim will be to avoid leakage, and we will find something like the linearly-hanned periodogram quite satisfactory.

On the other hand, if we deal with noise-like data with a reasonably flat spectrum our concern with statistical stability will be great. We may even be willing to use the raw periodogram, though this is rather unlikely.

The most frequent situation will call for both reasonable care in preserving statistical stability and reasonable care in avoiding leakage troubles.

If, for illustration, we were to convolve another short sequence of coefficients with the hanned a_k and hanned b_k, we will preserve the order of decay of minor lobes at $|\omega-\omega_k|^{-3}$, though the corresponding coefficient may well increase. Proper choice of such a sequence can restore, to the sums of successive modified periodogram values that are the natural estimates of the spectrum contribution from a frequency interval, most of the statistical stability that we lost when we hanned the a_k and b_k. Qualitatively, we have, using the equivalent description, multiplied the input data by a time function that 1) joins smoothly with zero at the ends of the data interval, 2) rises smoothly but moderately rapidly, and 3) is roughly level over most of the data. Some such data window appears to be the natural way to have and eat as much of our cake as possible—to combine statistical stability of sums with low leakage for individual terms.

VII. Interim Computational Recipes

We hope soon to know more about this balance, into which Sande has been looking actively. Until we have good reason to choose, however, we should proceed by judgment. Multiplying the data by a smooth function consisting of a short left-half cosine bell, a long constant and a right-half cosine bell seems today quite reasonable. If we make the half cosine bells each one tenth the length of the data, we may be making a reasonable compromise. For data stretching from $t=0$ to $t=T-1$, the formulas for such a data window would be

$$\left(\frac{1}{2}\right)\left(1-\cos\pi\frac{t}{0.1T}\right) \quad \text{for } 0 \le t \le 0.1T$$

$$1 \quad \text{for } 0.1T \le t \le 0.9T$$

$$\left(\frac{1}{2}\right)\left(1-\cos\pi\frac{T-t}{0.1T}\right) \quad \text{for } 0.9T \le t \le T, \quad \text{that is, } 0 \le T-t \le 0.1T.$$

Once we have applied this data window, we can add zeros to the ends of the data, make a fast Fourier transform, and calculate the raw Fourier periodogram of this modified time series, thus producing a modified periodogram of the original series as a basis for spectrum estimation.

In doing this, it will often be important to adjust the data, before windowing, to something close to mean zero and mean linear trend zero. Asking the half cosine bells to deal with large jumps can be quite unwise.

VIII. The Aims of Complex Demodulation

Complex demodulation can be considered to be a method of producing low-frequency "images" of more or less gross-frequency components of a time series. Computationally, each frequency band of interest is shifted to zero and the result run through a low-pass filter. If X_t is the original series, the frequency-shifted series is

$$\tilde{X}_t(\omega') = X_t e^{-it\omega'}$$

and the filtered complex demodulate is the complex-valued time series

$$Z_t(\omega') = \sum_{s=-m}^{m} a_s \tilde{X}_{t+s}(\omega').$$

(Retaining complex values is necessary to discriminate between $\omega'+\delta$ and $\omega'-\delta$ after the frequency shift.)

$Z_t(\omega')$, being complex, may also be expressed in polar form as

$$Z_t(\omega') = |Z_t(\omega')| e^{-i\phi_t(\omega')},$$

where $\phi_t(\omega')$ and $|Z_t(\omega')|$ are now the *phase* and *amplitude* (or *magnitude*) of $Z_t(\omega')$.

Properties of the series X_t, or of the process from which it comes, that are 1) local in frequency, and 2) smoothly changing over frequency, can be assessed or estimated in terms of the complex demodulates. For instance, if $f(\omega)$ is the spectrum density of X_t, then $f(\omega)\Delta\omega$ represents the variance assignable to the frequency band $(\omega-\Delta\omega/2, \omega+\Delta\omega/2)$, and can be estimated by an average of squared amplitudes of a corresponding complex demodulate (demodulated at ω). Similarly, cross spectra or higher-order poly spectra can be estimated from averages of products of complex demodulates from two or more series.

Such estimates as these are averages of time functions over the entire length of the series and thus estimate *time-global* properties of the series or process. Only in the case of stationarity will these also be *time-local* properties. However, even in the presence of nonstationarity, the behavior of individual values of the demodulates depends on relatively time-local properties of the series. Accordingly, time-local averages of complex demodulates can indicate or estimate such properties, showing up the existence or character of lack of stationarity, and providing bases for tests of the very hypothesis of stationarity itself.

An example of a time-local property is what can be called the "instantaneous phase" of the series at a particular frequency [12]. Suppose that there is a real "spike" in the spectrum of a time series caused by the presence of a strong semistable rhythm. In particular, consider the case when $X_t = C\cos(\omega t+\gamma)$. Frequency shifting down by $\omega' = \omega + \delta\omega$ will yield

$$\left(\frac{C}{2}\right)\exp\left[-i(\omega+\delta\omega)t\right] \cdot \left[\exp\left[i(\omega t+\gamma)\right] + \exp\left[-i(\omega t+\gamma)\right]\right]$$

$$= \left(\frac{C}{2}\right)\left(\exp\left[-i(t\cdot\delta\omega-\gamma)\right] + \exp\left[-i[(2\omega+\delta\omega)t+\gamma]\right]\right),$$

i.e., a signal containing frequencies $-\delta\omega$ and $2\omega+\delta\omega$. Hopefully, if our low-pass filter is any good, the component near 2ω will be eliminated and we will be left approximately with

$$Z_t(\omega+\delta\omega) = \left(\frac{C}{2}\right)A(-\delta\omega)\exp\left[-i(t\cdot\delta\omega+\gamma)\right],$$

where $A(\omega) = |A(\omega)/e^{i\phi(\omega)}$ is the transfer function of our low-pass filter. Thus,

$$\text{phase of } Z_t(\omega') = -(\delta\omega\cdot t+\gamma) + \phi(-\delta\omega)$$

which is linear in t with slope $-\delta\omega$, and can be used to estimate $\delta\omega$ and, hence, ω, the frequency of the underlying oscillation. More generally this suggests that it may be interesting to examine the phases of the complex demodulates, whether or not the data has a single underlying harmonic component. Noticing any identifiable pattern is likely to make it worth thinking about possible causes.

IX. Computational Approaches to Complex Demodulation

The most obvious procedure of computing complex demodulates is to work with the defining formulas, first explicitly shifting frequency by multiplying by a complex exponential and then filtering the result with suitably chosen filter weights a_j. A rough measure of the effort involved in an algorithm is the number of multiplies and adds needed. The number of (real) multiplies required to demodulate around a given frequency by the naive method is $2T+2(T-2m)(2m+1)+$(the cost of computing the exponentials, say $4T$) $\doteq 6T+4Tm$, and a comparable number of additions, where $2m+1$ is the length of the filter. This works out to be about $6+4m$ per original data point.

There are several ways to reduce the cost of computing demodulates.

1) Computing the values of a demodulate for all t is wasteful. Since these values have been low-pass filtered, you lose very little information by decimating them—by computing only every Dth value, say. And it seems clear that while D cannot be larger than m, it can probably be at least a modest fraction of m, say $D=m/\alpha$. If we compute only T/D values of our demodulate, we will need only $6T+2(T-2m)(2m+1)/D$ multiplies or approximately $6+4\alpha$ per original data point, which is likely to be much smaller than $6+4m$.

2) If we can be satisfied with a low-pass filter made up by several (say k) successive equal weight moving averages of length m_j, $j=1, \cdots, k$ (calculable as moving sums), we can replace multiplication by addition, passing from one moving sum to the next by adding one new value and subtracting one old one. We still have $6T$ multiplies to get the frequency-shifted series but only approximately $4kT$ adds, or about 6 multiplies and $4k$ adds per original data point. By the very nature of this algorithm we cannot gain by decimation. It should be pointed out that estimating the spectrum from complex demodulates filtered by a single moving average is equivalent to using a Bartlett window in the so-called indirect method, while two of the same length is the same as a Parzen window. (For more details see Appendix B.)

3) Low-pass filtering is essentially a convolution operation and, hence, the fast Fourier transform might be useful. The number of operations per data point is of the order $4\log_2 2m$. This is a great improvement over the naive approach for long filters.

4) Another and more fruitful approach to using the fast Fourier transform in complex demodulation is the following. Let us compute the fast Fourier transform of the entire time series, probably extended with zeroes. Instead of *smoothing* this as we did to obtain a modified periodogram, let us *multiply* it by a suitable discrete function of frequency centered, say at ω', and shift the result so that $\omega' \to 0$. Thus, if B_h are the values of the multiplying function and $c_k = \sum_t X_t e^{it\omega_k}$ are the original Fourier coefficients, the new coefficients (after shifting by $\omega' = \omega_k$) are $C_h^{(k)} = B_h c_{h+k}$. Let us now consider these coefficients as the Fourier coefficients of new time series, one for each k to be considered. Taking the inverse transform leads to

$$Z_t(\omega_k) = \sum_s b_s X_{t+s} \exp\left[-i(t+s)\omega_k\right],$$

where $b_s = \sum_k B_k \exp(is\omega_k)$. We recognize this complex time series as a complex demodulate at $\omega' = \omega_k$. So far we have really done nothing more than use the fast Fourier transform to convolve the time series with a filter as discussed before. However, by choosing B_j to be zero except over a relatively short band of frequencies we can do the inverse with a short and still cheaper transform, automatically obtaining a decimated series that ought to satisfy us, since it clearly contains all the information in the Fourier coefficients involved in its values. Thus, we can at once combine the computational superiority of the fast Fourier transform with the sensible practice of decimating the values of demodulates. (We will probably want to consider overlapping frequency bands in this process.)

A possible disadvantage of this method is the fact that we have replaced a transverse filter of limited extent with a circular filter extending over the entire time series. This is a familiar situation, except we are used to having it in the frequency domain, rather than in the time domain. We now worry about leakage across time, not frequency, but we are unlikely to need new ideas or concepts in arriving at sensible procedures.

Appendix I

Glossary

Time Series

Discrete time range: A finite number of equally spaced values of time.

Note 1: In all formulas, unless otherwise specified, there are T values of time, spaced one unit apart, starting with 0 and ending with $T-1$.

Discrete time series: An assignment of a numerical value X_t to each time t of a discrete time range.

Note 1: Unless otherwise specified the values of a discrete time series are real.

Continuous time range: A finite continuous interval of values of time.

Continuous time series: An assignment of a numerical value to each time of a continuous time range.

Note 1: In practice, any continuous time series is equivalent in every observable respect to a discrete time series consisting of sufficiently closely spaced values. Hence, all time series considered here are discrete.

Ideal (or Utopian) discrete-time stochastic process: A discrete-time stochastic process which 1) extends from $t = -\infty$ to $t = +\infty$, 2) has finite variance (for each t), and 3) is second-order stationary.

Attainable discrete-time stochastic process: A discrete-time stochastic process defined for (only) a (finite) discrete time range.

Noise: A time series in which it is most fruitful to consider the values as random variables. Repetitions of such a time series under essentially identical conditions need have only statistically definable properties in common.

Signal: A time series whose values are probably most usefully regarded as nonrandom, in the sense that a repetition under essentially identical conditions would yield essentially the same series.

Note 1: The difference between *noise* and *signal* can, sometimes usefully, be regarded as a difference in what we regard as "essentially identical conditions."

Operations on a Time Series

Data window: A function of discrete time by which a time series is multiplied.

Note 1: The use of a data window is often very appropriate before Fourier transformation, or before other processes that could conveniently begin with a Fourier transformation.

Convolution of two finite sequences: The sequence

$$Z_t = \sum_s X_s Y_{t-s},$$

where t varies over all values for which the sum is nonempty, and where each sum is over all s for which the summand is defined.

Transfer function of a filter: The output of a linear filter operating on the time series $X_t = \cos(\omega t + \gamma)$ has the form $T_t = |A(\omega)| \cos[\omega t + \gamma + \phi(\omega)]$. The complex-valued function of angular frequency ω, $A(\omega) = |A(\omega)| \exp[i\phi(\omega)]$, is the transfer function of the filter.

Note 1: The transfer function of the transverse filter,

$$Y_t = \sum_s a_s X_{t+s} \quad \text{is} \quad A(\omega) = \sum_s a_s e^{is\omega}.$$

Fourier Transforms of a Discrete Time Series

The (continuous) Fourier transform of a discrete time series: The complex-valued function of (angular) frequency ω

$$X(\omega) = \sum_{t=0}^{T-1} X_t \cdot \exp(it\omega).$$

Note 1: $X(\omega)$ is always periodic with period 2π.

Note 2: If the X_t are real, $X(-\omega)=[X(\omega)]^*$ (complex conjugate), and the continuous Fourier transform is determined by its values for $0\leq\omega\leq\pi$.

Note 3: The continuous Fourier transform is of theoretical importance only, helping to unify both discussions and insight.

The (unnormalized) Fourier coefficients of a discrete time series: The T complex numbers

$$a_k + ib_k = X\left(2\pi\frac{k}{T}\right), \quad k = 0, \cdots, T-1.$$

Note 1: Because of the periodicity of the Fourier transform, we could define Fourier coefficients for negative frequencies as

$$a_{-k} + ib_{-k} = X\left(2\pi\frac{T-k}{T}\right) = a_{T-k} + ib_{T-k}.$$

Note 2: If X_t is real, $a_{T-k}=a_k$ and $b_{T-k}=-b_k$. Hence, $b_0=0$, and, if T is even, $b_{T/2}=0$. Thus, all Fourier coefficients can be determined from the coefficients of the first $(T+1)/2$ (T odd) or $(T+2)/2$ (T even) frequencies. These contain exactly T (nonidentically vanishing) real numbers. Suitably normalized these T real numbers $(a_0, a_1, b_1, \cdots)$ are an orthogonal transform of the (real) X_t.

Note 3: If X_t is complex, all T frequencies are needed and all coefficients are, in general, genuinely complex. Suitably normalized, the $2T$ a_k and b_k are an orthogonal transform of the $2T$ real and imaginary parts of X_t.

Note 4: (inverse transform) If $Y_k=a_k-ib_k$ (note sign), then the X_t can be found from the Fourier coefficients of Y_k as

$$X_t = \frac{1}{T}Y\left(2\pi\frac{t}{T}\right)^* \quad (\text{* means complex conjugate}).$$

Note 5: If X_t is real, then $X_t=(1/T)\ Y(2\pi\ t/T)$.

Hyper-Fourier coefficients of a discrete time series: If a discrete time series is extended to a time series of length $S\geq T$ by adding zeros at its ends, the Fourier coefficients of the extended series are a set of hyper-Fourier coefficients of the original time series.

The fast Fourier transform: An algorithmic process for calculating with great computational efficiency the Fourier coefficients of a given series, provided the number of values given has many small factors.

Note 1: The algorithm used makes particular use of the structure of $\{e^{2\pi itk/T}\}$, for t variable and k a parameter (or vice versa), and requires on the order of $2T\log_2 T$ arithmetic operations when T is a power of 2. (Naive calculations require T^2 or $T^2/2$ arithmetic operations. For more details see Appendix III).

Periodogram of a Discrete Time Series

Continuous periodogram of a discrete time series: The real-valued function of angular frequency ω

$$P(\omega) = \left(\frac{1}{T}\right)\left|\sum_{t=0}^{T-1} X_t \exp(it\omega)\right|^2.$$

Note 1: $P(\omega)$ is proportional to the squared modulus of the (continuous) Fourier transform of X_t.

Note 2: A useful relation if X_t is real is

$$P(\omega) = \sum_{t=-T+1}^{T-1} \hat{C}_t \cos t\omega,$$

where

$$\hat{C}_t = \left(\frac{1}{T}\right)\sum_{s=0}^{T-t-1} X_s X_{s+t}, \quad t \geq 0,$$

and

$$\hat{C}_t = \hat{C}_{-t} \quad \text{for } t \leq 0.$$

The (raw) Fourier periodogram of a discrete time series: The sequence of values $(a_k^2+b_k^2)/T$ (attached to frequency $\omega=2\pi k/T$) where the a_k+ib_k are the Fourier coefficients of the time series.

Note 1: The values of the Fourier periodogram are also given by $P(2\pi k/T)$, where $P(\omega)$ is the continuous periodogram of X_t.

Modified Fourier periodogram of a discrete time series: If the Fourier coefficients of a discrete time series, possibly extended with zeros, are smoothed *before* squaring, the resulting function of (discrete) angular frequency is a modified periodogram.

Note 1: The same modified periodogram can be obtained by multiplying the given time series, possibly extended with zeros, by a suitable data window, and then forming the raw periodogram of the modified series.

Note 2: For example,

$$P'(\omega_k) = (1/T)\,|\tilde{X}(\omega_k)|^2,$$

where

$$\tilde{X}(\omega_k) = -(1/4)X(\omega_{k-1}) + (1/2)X(\omega_k) - (1/4)X(\omega_{k+1}),$$

is the modified periodogram obtained by simple hanning of $X(\omega)$ (in the form appropriate for a series beginning at $t=0$ rather than centered there). The equivalent data window is proportional to $(1/2)(1-\cos 2\pi t/T)$.

Note 3: A modified periodogram is *not* to be confused with, and cannot be obtained as, the result of smoothing a (raw) periodogram.

Spectrum of a Time Series

Spectrum as a general concept: An expression of the contribution of frequency ranges to the mean-square size, or to the variance, of a single time function or of an ensemble of time functions.

Spectrum of an ideal discrete-time stochastic process: The relations

$$\text{ave}\,\{X_t X_{t+s}\} = \int_0^\pi \cos s\omega dS_0(\omega), \qquad s = 0, 1, 2, \cdots$$

and

$$\text{cov}\,\{X_t, X_{t+s}\} = \int_0^\pi \cos s\omega dS(\omega), \qquad s = 0, 1, 2, \cdots$$

define, for any real ideal discrete-time stochastic process, essentially unique increasing functions $S_0(\omega)$ and $S(\omega)$ for $0- \leq \omega \leq \pi +$. S_0 or, better, S, is conventionally taken to represent the (unnormalized) cumulative spectrum of the process.

Note 1: Sometimes, especially when ω is allowed to run from $-\pi$ to $+\pi$, (1/2) S_0 or (1/2) S is so taken.

Note 2: The derivative $dS_0(\omega)/d\omega$ or $dS(\omega)/d\omega$, when it exists, is the (unnormalized) spectrum density.

Spectrum of an attainable discrete-time stochastic process over a fixed interval: Let I be a time interval of integer length $|I|$. Let $\sum_{t \text{ in } I}$ be a sum over integers or "half integers" with half weight when t is an endpoint of I. Let

$$R(s) = \left(\frac{1}{|I|}\right) \sum_{t \text{ in } I} \text{cov}\,\{X_{t+s/2}, X_{t-s/2}\}, \qquad s = 0, \cdots, |I| - 1$$

$$R(s) = \int_0^\pi \cos s\omega dS(\omega), \quad s = 0, \cdots, |I| - 1,$$

where X_t is a real attainable discrete-time stochastic process. Then *any* $S(\omega)$ such that

$$R(s) = \int_0^\pi \cos s\omega dS(\omega), \quad s = 0, \cdots, |I| - 1,$$

is said (by us) to be a cumulative spectrum for the process, averaged over the time interval I.

Cosine polynomial principle: The theorem that any homogeneous quadratic function Q of the observations has an average value of the form

$$\text{ave}\,\{Q\} = \int_0^\pi q(\omega) dS(\omega) + q(0)(\text{ave}\{X_t\})^2 = \int_0^\pi q(\omega) dS_0(\omega)$$

for every real ideal discrete-time stochastic process, where $q(\omega)$ is a polynomial in $\cos \omega$ of degree no greater than the greatest difference in subscripts in the X's entering Q.

Spectrum estimate: A homogeneous quadratic function Q is said, for every ideal discrete-time stochastic process, to estimate the spectrum (density) $dS(\omega)/d\omega$ weighted by $q(\omega)$, where $q(\omega)$'s existence is asserted by the cosine polynomial principle.

Note 1: If Q is a linear combination of a selected set of special quadratics, such as

$$\frac{1}{|I|} \sum_{t \text{ in } I} X_{t+s/2} X_{t-s/2},$$

or alternatively,

$$\frac{1}{|I|} \sum_{t \text{ in } I} (X_{t-s/2} - X_{t+s/2})^2,$$

then it is said (by us) to estimate the corresponding weighted spectrum, whether or not the process is second-order stationary.

Leakage into a spectrum estimate: A phenomenon by which the value of a spectrum estimate, which was intended to estimate a weighted average of the spectrum over a specific frequency interval, is affected by components of more or less remote frequencies outside the interval.

Appendix II

Complex Demodulation Without the Fast Fourier Transform

Review of Developments

Calculations of power spectrum estimates that move directly from observed data (probably multiplied by a data window) to a function (or functions) of frequency without intermediate calculation of other time-domain functions (such as correlograms or mean lagged products) are instances of *direct estimation.* Direct estimation has been carried out for many years through the use of special purpose analog devices (harmonic analyzers, filter banks, wave analyzers, etc.). For the earlier general purpose computers and before the arrival of disks and large memories, it seemed that direct estimation would be less efficient than going through mean lagged products. However, both hardware and algorithm have changed rapidly, so that today the choice of method depends more on the objectives of the analysis than on technical limitations.

Although most of the steps involved in direct digital spectrum estimation without fast Fourier transform have been studied in connection with digital filtering, their incorporation into more or less general purpose computer programs has been very recent [2], [13], and [15]. Computations using the procedures described below have been performed both on an IBM 7094 [2] and on an IBM 1620, Model 1 [13]. The large storage requirements of this method make the use of disk practically essential with either machine, but the size of the machine (i.e., at the main frame) has proved unimportant.

se of Complex Demodulation

The direct method of spectrum estimation using ›mplex demodulates is as follows:

If X_t, $t=0, \cdots, T-1$, is a time series, a complex ›modulate at (angular) frequency ω' is the complex me series

$$Z_t(\omega') = \sum_{t=-m}^{+m} a_s X_{t+s} e^{-i\omega'(t+s)},$$

here a_s, $s=-m, \cdots, m$, are the weights of a (usually ›mmetrical) low-pass filter. First the frequency content : the series is shifted down by ω' by multiplying by the ›mplex exponential, and then the result is low-pass ltered. The result $Z_t(\omega')$ should then be a "low-equency image" of that part of X_t which can be asso-ated with variations at or near frequency ω'. (One oint to be noted is that the process of filtering has eprived us of m observations at each end of the series,) that $Z_t(\omega')$ is completely defined only for $t=m, \cdots,$ '$-m-1$.) The natural estimate of the (averaged) spec-·um near ω' is then

$$f(\omega') = \left(\frac{1}{T-2m}\right) \sum_{t=m}^{T-m-1} |Z_t(\omega')|^2.$$

:elation to the Mean-Lagged-Product Route

We can rearrange the complex-demodulate estimate › yield

$$\left(\frac{1}{T-2m}\right) \sum_{t=m}^{T-m-1} |Z_t(\omega')|^2$$
$$= \sum_{s_1=-m}^{m} \sum_{s_2=-m}^{m} a_{s_1} a_{s_2} e^{i(s_1-s_2)\omega'} \frac{1}{T-2m} \sum_{t=m}^{T-m-1} X_{t+s_1} X_{t+s_2}.$$

'or each value of s_1 and s_2 appearing in the outer sums, he innermost sum is a mean of lagged products at lag $_1-s_2$. In general, all these sums for a given lag s will iffer. However, if the X_t series begins and ends with at ›ast $2m$ zeros (i.e., $X_0=X_1=\cdots=X_{m-1}=X_{T-2m}=\cdots=X_{T-1}=0$), then

$$\left(\frac{1}{T-2m}\right) \sum_{t=m}^{T-m-1} X_{t+s_1} X_{t+s_1+s}$$
$$= \left(\frac{1}{T}\right)\left(\frac{T}{T-2m}\right) \sum_{t=0}^{T-s-1} X_t X_{t+s}$$
$$= \left(\frac{T}{T-2m}\right) \hat{C}(s).$$

[he complex-demodulate estimate of the spectrum is, ınder these circumstances, given by

$$\sum_{s_1} \sum_{s_2} a_{s_1} a_{s_2} e^{i(s_1-s_2)\omega'} \left(\frac{T}{T-2m}\right) \hat{C}(s_1 - s_2)$$
$$= \frac{T}{T-2m} \sum_s b_s e^{is\omega'} \hat{C}(s),$$

where

$$b_s = \sum_{s_1+s_2=s} a_{s_1} a_{s_2}.$$

The conventional mean-lagged-product estimate is (in one of the preferred forms)

$$\sum_s b_s e^{is\omega'} \hat{C}(s) = \sum_{s_1} \sum_{s_2} a_{s_1} a_{s_2} e^{i(s_1-s_2)\omega'} \hat{C}(s).$$

One way of describing the above algebraic identity is to remark that the use of the mean-lagged-product estimate is equivalent to including in the complex-demodulate estimate all possible output values of the low-pass filter, even those which are incomplete because of "end effects." For large T the effect of including or excluding these is negligible and the two methods are effectively identical.

Bandwidth and Stability

However, if we estimate a spectrum as a quadratic function of the data (the best we can do is to estimate "on the average" the result of weighting the spectrum by a well-chosen cosine polynomial) there is inevitably a question of compromise between narrow bandwidth and high statistical stability. Much has been written, some helpfully, on this point. For large T, as we noticed above, the use of complex demodulates is essentially equivalent to the use of mean lagged products with a matched window. Accordingly, all the usual discussion applies to estimation by complex demodulates (as it does for less simple reasons for even moderate values of T). For the form of filter discussed in the text [i.e., k successive equal-weight moving averages of length $(2m/k)+1$], the spectrum window is

$$B_k(\omega) = \left[\frac{\sin (m/k)\omega}{(m/k) \sin \omega}\right]^{2k},$$

and the effective degrees of freedom are

$$2\left[\int_0^\pi B_k(\omega)d\omega\right]^2 \Big/ \int_0^\pi B_k^2(\omega)d\omega$$
$$= 2k(T - 2m + 1)/(2m + 1).$$

Appendix III

The Fast Fourier Transform

The Basic Idea

The fast Fourier transform is any one of a class of highly efficient algorithms for computing the complex Fourier coefficients of a discrete (time) series X_t, $t=0, \cdots, T-1$, when T is highly composite (has many small factors). (Its history is sketched in Section III.) It is primarily a complex (discrete) Fourier transform for *complex* X_t and will be discussed as such. In counting operations, etc., we shall at first be referring to complex operations.

The basic idea can be illustrated in the case when T has two factors, say $T=p_1p_2$. The complex Fourier coefficient at frequency $\omega_m=2\pi m/T$ is

$$X(\omega_m) = \sum_{t=0}^{T-1} X_t e^{2\pi i (tm/T)}$$

$$= \sum_{u_1=0}^{p_1-1} \sum_{u_2=0}^{p_2-1} X_{u_1+u_2p_1} \exp\left(2\pi i (u_1 + u_2 p_1) \frac{m}{p_1p_2}\right)$$

$$= \sum_{u_1=0}^{p_1-1} \exp\left(2\pi i u_1 \frac{m}{p_1p_2}\right) \cdot \sum_{u_2=0}^{p_2-1} X_{u_1+u_2p_1} \exp\left(2\pi i u_2 \frac{m}{p_2}\right).$$

In a similar way as we have decomposed t in terms of p_1 and p_2, so can we express m as $m=U_1p_2+U_2$, where $0\le U_1 \le p_1-1$ and $0 \le U_2 \le p_2-1$. Using this decomposition the sum reduces to

$$\sum_{u_1=0}^{p_1-1} \exp\left(2\pi i u_1 \frac{U_1p_2+U_2}{p_1p_2}\right) \cdot \sum_{u_2=0}^{p_2-1} X_{u_1+u_2p_1} \exp\left(2\pi i u_2 \frac{U_2}{p_2}\right).$$

(Note the cancelling in the innermost complex exponential.) The inner sum is of length p_2 and need be evaluated for only p_1 different values of u_1 and p_2 different values of U_2, requiring $p_2 \cdot p_1p_2$ multiplies in all. Having computed all possible values of the inner sum, the outer sum, of length p_1, needs to be computed for p_1 values of U_1 and p_2 values of U_2, using $p_1 \cdot p_1p_2$ multiplies. Thus, evaluation of the Fourier transform at all $p_1p_2=T$ Fourier frequencies requires $(p_1+p_2)p_1p_2=(p_1+p_2)T$ multiplies. Naive calculation requires T^2 multiplies. Note that the inner sum represents, when we hold u_1 constant and let U_2 vary, a Fourier transform of length p_2. If $T=p_1p_2, \cdots, p_r$, then $(p_1+p_2+\cdots+p)T$ multiplies suffice. In particular, if $T=2^n$, we can compute the complete set of Fourier coefficients using $2nT=2T\log_2 T$ multiplies. If $T=1024=2^{10}$, then $2T \log_2 T=20\,480$ while $T^2=1\,048\,576$ which is more than 50 times 20 480.

The C-T and S-T Algorithms

There are at least two somewhat different algorithmic approaches to implementing the fast Fourier transform, one due to Cooley and Tukey (the C-T method) [8], and another (the S-T method) programmed by Sande [14] along lines suggested in lectures by Tukey. We shall treat both, hoping to clarify the relationship between them and, as well, to gain familarity with and understanding of what is really going on in the fast Fourier transform.

We shall use the very useful notation employed by Sande

$$e(f) = \exp(2\pi i f).$$

With this notation, the transform to be computed is

$$X(\omega_m) = \sum_{t=0}^{T-1} e(tm/T)X_t, \quad m = 0, \cdots, T-1.$$

Suppose, $T=p_1p_2, \cdots, p_r=p_rp_{r-1}, \cdots, p_1$ ($p_j>1$, but not necessarily prime), then there are two natural ways to decompose any integer $<T$ into "digits" in a (possibly) compound scale of notation.

$$1)\ t = u_1 + u_2p_1 + \cdots + u_rp_1p_2\cdots p_{r-1}$$
$$= u_1 + u_2\Pi_1 + \cdots + u_r\Pi_{r-1},$$

and

$$2)\ m = U_r + U_{r-1}p_r + U_{r-2}p_rp_{r-1} + \cdots + U_1p_r\cdots p_2$$
$$= \left(\frac{U_r}{\Pi_r} + \cdots + \frac{U_1}{\Pi_1}\right)\Pi_r.$$

For convenience later we introduce the following notation for truncated sections of m and t

$$t_{(j)} = (\text{first } j \text{ terms of } t)$$
$$= u_1 + u_2\Pi_1 + \cdots + u_j\Pi_{j-1}$$

and

$$m_{(j)} = (\text{first } r-j+1 \text{ terms of } m)$$
$$= \left(\frac{U_r}{\Pi_r} + \cdots + \frac{U_j}{\Pi_j}\right)\Pi_r.$$

In words, the u_j are the "digits," in *reverse order*, when t is written in the compound scale of notation in which p_r goes with the left-hand digit, while $t_{(j)}$ corresponds to the lowest j of these digits. Analogously, the U_j are the "digits," *in normal order*, when m is written in the compound scale of notation in which p_1 goes with the left-hand digit, while $m_{(j)}$ corresponds to the lowest $r-j+1$ of these digits.

The Working Identities

The key to the C-T and S-T methods lies in the following identities, which make strong use of the fact that $e(f+g)=e(f)$ whenever g is an integer

$$e(tm/T) = e\left[\sum_{k=1}^{r} u_k\Pi_{k-1} \sum_{j=1}^{r}\left(\frac{U_j}{\Pi_j}\right)\right]$$

$$= e\left[\sum_{k=1}^{r} u_k \sum_{j=k}^{r} U_j \frac{\Pi_{k-1}}{\Pi_j}\right] \qquad (C\text{-}T)$$

$$= e\left[\sum_{j=1}^{r} U_j \sum_{k=1}^{j} u_k \frac{\Pi_{k-1}}{\Pi_j}\right] \qquad (S\text{-}T).$$

The first important step in the fast Fourier transform is the following identity

$$\sum_{t=0}^{T-1} e(tm/T)X_t = \sum_{u_1=0}^{p_1-1} \cdots \sum_{u_r=0}^{p_r-1} e(tm/T)X_t.$$

Using the C-T identity, this is seen to be equivalent to

$$\sum_{u_1=0}^{p_1-1} e\left[u_1 \sum_{j=1}^{r} \frac{U_j}{\Pi_j}\right] \sum_{u_2=0}^{p_2-1} e\left[u_2\Pi_1 \sum_{j=2}^{r} \frac{U_j}{\Pi_j}\right] \cdots$$
$$\sum_{u_r=0}^{p_r-1} e\left[u_r\Pi_{r-1} \frac{U_r}{\Pi_r}\right] X_{u_1+u_2\Pi_1+\cdots+u_r\Pi_{r-1}}$$
$$= \sum_{u_1=0}^{p_1-1} e\left(u_1\frac{U_1}{p_1}\right)\left[e\left(u_1\frac{m_{(2)}}{T}\right) \sum_{u_2=0}^{p_2-1} e\left(u_2\frac{U_2}{p_2}\right)\right.$$
$$\cdot\left[e\left(u_2\frac{m_{(3)}}{T}\right) \cdots \left[e\left(u_{r-1}\frac{m_{(r)}}{T}\right) \sum_{u_r=0}^{p_r-1}\right.\right.$$
$$\left.\left.\left.\cdot e\left(u_r\frac{U_r}{p_r}\right) X_{u_1+u_2\Pi_1+\cdots+u_r\Pi_{r-1}}\right] \cdots\right]\right].$$

The S-T decomposition of $\sum_{t=0}^{t-1} e(m/T)X_t$ leads to

$$\sum_{u_1=0}^{p_1-1} e\left(U_1\frac{u_1}{p_1}\right) \sum_{u_2=0}^{p_2-1} e\left[U_2 \sum_{k=1}^{2} u_k\frac{\Pi_{k-1}}{\Pi_2}\right] \cdots$$
$$\sum_{u_r=0}^{p_r-1} e\left[U_r \sum_{k=1}^{r} u_k\frac{\Pi_{k-1}}{\Pi_r}\right] X_{u_1+u_2\Pi_1+\cdots+u_r\Pi_{r-1}}$$
$$= \sum_{u_1=0}^{p_1-1} e\left(u_1\frac{U_1}{p_1}\right)\left[e\left(U_2\frac{t_{(1)}}{\Pi_2}\right) \sum_{u_2=0}^{p_2-1} e\left(u_2\frac{U_2}{\Pi_2}\right)\right.$$
$$\cdot\left[e\left(U_3\frac{t_{(2)}}{\Pi_3}\right) \cdots \left[e\left(U_r\frac{t_{(r-1)}}{\Pi_2}\right) \sum_{u_r=0}^{p_r-1}\right.\right.$$
$$\left.\left.\left.\cdot e\left(u_r\frac{U_r}{p_r}\right) X_{u_1+u_2\Pi_1+\cdots+u_r\Pi_{r-1}}\right] \cdots\right]\right].$$

Comparison of the Algorithms

The C-T and S-T equations are almost identical in form. At the jth stage, $p_1p_2 \cdots p_r/p_j = T/p_j$, discrete Fourier transforms of length p_j are needed. The T values thus computed are then multiplied by a factor which takes the forms $e(u_{j-1}m_{(j)}/T)$ (for C-T) or $e(U_jt_{(j-1)}/\Pi_j)$ (for S-T). The ease of using each method depends on the ease of finding these factors. (It may sometimes be advantageous to bring the factors inside the adjacent summation, but the problem of computing them remains.) The primary advantage of the S-T factor is that the integer $t_{(j)}$ is already needed to find the storage location of the value which the factor multiplies. The relation of this location to $m_{(j)}$ is more indirect, requiring, in the case when all $p_k=2$, a bit reversal. Thus, unless the data should be stored in an abnormal form, the S-T method seems algorithmically more simple. This conclusion is valid when the Fourier transform is computed "in place." By copying back and forth between two storage areas, the advantage of the S-T algorithm disappears.

Both methods lead to an array of Fourier coefficients in a very scrambled form (when computed "in place"). The coefficient corresponding to $m = U_r + U_{r-1}p_r + \cdots + U_1p_r \cdots p_2$ ends up in the location which was originally occupied by $X_{U_1+U_2p_1+\cdots+U_rp_1\cdots p_{r-1}}$. In the case when $p_1 = p_2 = \cdots = p_r$, the "unscrambling" can easily be done in place. In other cases it seems at present to be necessary to do some copying.

Use of the Algorithm

The fast Fourier transform as it is programmed (by Sande using the S-T algorithm) and available at Princeton University has as input a formal series of length $T=2^n$ with real and imaginary parts in two separate arrays. The program replaces the real and imaginary parts of the data with the (unscrambled) real and imaginary parts of the transform. If one has real data there are (at least) three ways to proceed, taking advantage of the relationship $X(\omega_k) = [X(\omega_{T-k})]^*$.

1) *Raw use* (wasteful of both storage space and operations): Use the raw transform with the actual (real) input in the real-part array and zeros in the imaginary-part array. This requires storage of length $2T$ and produces $2T$ components of T complex Fourier coefficients of which only T are needed [say for subscripts up to $(T+1)/2$ or $(T+2)/2$].

2) *Dual use* [efficient when two series of (nearly) equal length are to be transformed for *any* purpose]: If we have two real series X_t and Y_t we can perform the raw fast Fourier transform on $Z_t = X_t + iY_t$. Then

$$X(\omega_k) = \mathrm{Re}\,[(Z(\omega_k) + Z(\omega_{T-k}))/2] + i\,\mathrm{Im}\,[(Z(\omega_k) - Z(\omega_{T-k}))/2]$$

and

$$Y(\omega_k) = \mathrm{Im}\,[(Z(\omega_k) + Z(\omega_{T-k}))/2] - i\,\mathrm{Re}\,[(Z(\omega_k) - Z(\omega_{T-k}))/2]$$

suffice to give the $2T$ components of the two sets of Fourier coefficients involving the first $(T+1)/2$ or $(T+2)/2$ frequencies.

3) *Odd-even use* (almost a special case of 2) above): If T is even, consider the identity

$$X(\omega_k) = \sum_{t=0}^{T-1} e(tk/T)X_t = \sum_{s=0}^{(T/2)-1} e(2sk/T)X_{2s} + e(k/T)\sum_{s=0}^{(T/2)-1} e(2sk/T)X_{2s+1}$$
$$= \sum_{s=0}^{(T/2)-1} e(sk/(T/2))X_{2s} + e(k/T)\sum_{s=0}^{(T/2)-1} e(sk/(T/2))X_{2s+1}$$

whose last form is essentially the invention made by Danielson and Lanczos [5]. (This is actually a particular case of an identity used earlier.) Thus, we see the transform of length T can be found from two length $T/2$ transforms on the two (real) series $X_0, X_2, \cdots, X_{T-2}$ and $X_1, X_3, \cdots, X_{T-1}$. Provided we can manage to split the series up this way, we can compute the two transforms using method 2) above and recombine them together with the complex exponential. The splitting (in place) has been programmed (by Bingham) taking advantage of the decomposition into disjoint cycles of the permutation to which it is equivalent.

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