CITED REFERENCES AND FURTHER READING:

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13.8 Spectral Analysis of Unevenly Sampled Data

Thus far, we have been dealing exclusively with evenly sampled data,

$$h_n = h(n\Delta)$$
 $n = \dots, -3, -2, -1, 0, 1, 2, 3, \dots$ (13.8.1)

where Δ is the sampling interval, whose reciprocal is the sampling rate. Recall also (§12.1) the significance of the Nyquist critical frequency

$$f_c \equiv \frac{1}{2\Delta} \tag{13.8.2}$$

as codified by the sampling theorem: A sampled data set like equation (13.8.1) contains *complete* information about all spectral components in a signal h(t) up to the Nyquist frequency, and scrambled or *aliased* information about any signal components at frequencies larger than the Nyquist frequency. The sampling theorem thus defines both the attractiveness, and the limitation, of any analysis of an evenly spaced data set.

There are situations, however, where evenly spaced data cannot be obtained. A common case is where instrumental drop-outs occur, so that data is obtained only on a (not consecutive integer) subset of equation (13.8.1), the so-called *missing data* problem. Another case, common in observational sciences like astronomy, is that the observer cannot completely control the time of the observations, but must simply accept a certain dictated set of t_i 's.

There are some obvious ways to get from unevenly spaced t_i 's to evenly spaced ones, as in equation (13.8.1). Interpolation is one way: lay down a grid of evenly spaced times on your data and interpolate values onto that grid; then use FFT methods. In the missing data problem, you only have to interpolate on missing data points. If a lot of consecutive points are missing, you might as well just set them to zero, or perhaps "clamp" the value at the last measured point. However, the experience of practitioners of such interpolation techniques *is not reassuring*. Generally speaking, such techniques perform poorly. Long gaps in the data, for example, often produce a spurious bulge of power at low frequencies (wavelengths comparable to gaps).

A completely different method of spectral analysis for unevenly sampled data, one that mitigates these difficulties and has some other very desirable properties, was developed by Lomb [1], based in part on earlier work by Barning [2] and Vaníček [3], and additionally elaborated by Scargle [4]. The Lomb method (as we will call it) evaluates data, and sines and cosines, only at times t_i that are actually measured. Suppose that there are N data points $h_i \equiv h(t_i), i = 1, ..., N$. Then first find the mean and variance of the data by the usual formulas,

$$\overline{h} \equiv \frac{1}{N} \sum_{i=1}^{N} h_{i} \qquad \sigma^{2} \equiv \frac{1}{N-1} \sum_{i=1}^{N} (h_{i} - \overline{h})^{2}$$
 (13.8.3)

Now, the Lomb normalized periodogram (spectral power as a function of angular frequency $\omega \equiv 2\pi f > 0$) is defined by

$$P_N(\omega) \equiv \frac{1}{2\sigma^2} \left\{ \frac{\left[\sum_j (h_j - \overline{h}) \cos \omega(t_j - \tau)\right]^2}{\sum_j \cos^2 \omega(t_j - \tau)} + \frac{\left[\sum_j (h_j - \overline{h}) \sin \omega(t_j - \tau)\right]^2}{\sum_j \sin^2 \omega(t_j - \tau)} \right\}$$
(13.8.4)

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Here τ is defined by the relation

$$\tan(2\omega\tau) = \frac{\sum_{j} \sin 2\omega t_{j}}{\sum_{j} \cos 2\omega t_{j}}$$
(13.8.5)

The constant τ is a kind of offset that makes $P_N(\omega)$ completely independent of shifting all the t_i 's by any constant. Lomb shows that this particular choice of offset has another, deeper, effect: It makes equation (13.8.4) identical to the equation that one would obtain if one estimated the harmonic content of a data set, at a given frequency ω , by linear least-squares fitting to the model

$$h(t) = A\cos\omega t + B\sin\omega t \tag{13.8.6}$$

This fact gives some insight into why the method can give results superior to FFT methods: It weights the data on a "per point" basis instead of on a "per time interval" basis, when uneven sampling can render the latter seriously in error.

A very common occurrence is that the measured data points h_i are the sum of a periodic signal and independent (white) Gaussian noise. If we are trying to determine the presence or absence of such a periodic signal, we want to be able to give a quantitative answer to the question, "How significant is a peak in the spectrum $P_N(\omega)$?" In this question, the null hypothesis is that the data values are independent Gaussian random values. A very nice property of the Lomb normalized periodogram is that the viability of the null hypothesis can be tested fairly rigorously, as we now discuss.

The word "normalized" refers to the factor σ^2 in the denominator of equation (13.8.4). Scargle [4] shows that with this normalization, at any particular ω and *in the case of the null hypothesis*, $P_N(\omega)$ has an exponential probability distribution with unit mean. In other words, the probability that $P_N(\omega)$ will be between some positive z and z + dz is $\exp(-z)dz$. It readily follows that, if we scan some M *independent* frequencies, the probability that none give values larger than z is $(1 - e^{-z})^M$. So

$$P(>z) \equiv 1 - (1 - e^{-z})^M \tag{13.8.7}$$

is the false-alarm probability of the null hypothesis, that is, the *significance level* of any peak in $P_N(\omega)$ that we do see. A small value for the false-alarm probability indicates a highly significant periodic signal.

To evaluate this significance, we need to know M. After all, the more frequencies we look at, the less significant is some one modest bump in the spectrum. (Look long enough, find anything!) A typical procedure will be to plot $P_N(\omega)$ as a function of many closely spaced frequencies in some large frequency range. How many of these are independent?

Before answering, let us first see how accurately we need to know M. The interesting region is where the significance is a small (significant) number, $\ll 1$. There, equation (13.8.7) can be series expanded to give

$$P(>z) \approx M e^{-z} \tag{13.8.8}$$

We see that the significance scales linearly with M. Practical significance levels are numbers like 0.05, 0.01, 0.001, etc. An error of even $\pm 50\%$ in the estimated significance is often tolerable, since quoted significance levels are typically spaced apart by factors of 5 or 10. So our estimate of M need not be very accurate.

Horne and Baliunas [5] give results from extensive Monte Carlo experiments for determining M in various cases. In general M depends on the number of frequencies sampled, the number of data points N, and their detailed spacing. It turns out that M is very nearly equal to N when the data points are approximately equally spaced, and when the sampled frequencies "fill" (oversample) the frequency range from 0 to the Nyquist frequency f_c (equation 13.8.2). Further, the value of M is not importantly different for random spacing of the data points than for equal spacing. When a larger frequency range than the Nyquist range is sampled, M increases proportionally. About the only case where M differs significantly from the case of evenly spaced points is when the points are closely clumped, say into groups of 3; then (as one would expect) the number of independent frequencies is reduced by a factor of about 3.

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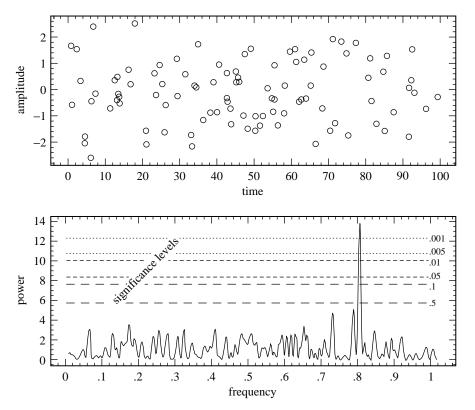


Figure 13.8.1. Example of the Lomb algorithm in action. The 100 data points (upper figure) are at random times between 0 and 100. Their sinusoidal component is readily uncovered (lower figure) by the algorithm, at a significance level better than 0.001. If the 100 data points had been evenly spaced at unit interval, the Nyquist critical frequency would have been 0.5. Note that, for these unevenly spaced points, there is no visible aliasing into the Nyquist range.

The program period, below, calculates an effective value for M based on the above rough-and-ready rules and assumes that there is no important clumping. This will be adequate for most purposes. In any particular case, if it really matters, it is not too difficult to compute a better value of M by simple Monte Carlo: Holding fixed the number of data points and their locations t_i , generate synthetic data sets of Gaussian (normal) deviates, find the largest values of $P_N(\omega)$ for each such data set (using the accompanying program), and fit the resulting distribution for M in equation (13.8.7).

Figure 13.8.1 shows the results of applying the method as discussed so far. In the upper figure, the data points are plotted against time. Their number is N = 100, and their distribution in t is Poisson random. There is certainly no sinusoidal signal evident to the eye. The lower figure plots $P_N(\omega)$ against frequency $f = \omega/2\pi$. The Nyquist critical frequency that would obtain if the points were evenly spaced is at $f = f_c = 0.5$. Since we have searched up to about twice that frequency, and oversampled the f's to the point where successive values of $P_N(\omega)$ vary smoothly, we take M = 2N. The horizontal dashed and dotted lines are (respectively from bottom to top) significance levels 0.5, 0.1, 0.05, 0.01, 0.005, and 0.001. One sees a highly significant peak at a frequency of 0.81. That is in fact the frequency of the sine wave that is present in the data. (You will have to take our word for this!)

Note that two other peaks approach, but do not exceed the 50% significance level; that is about what one might expect by chance. It is also worth commenting on the fact that the significant peak was found (correctly) *above the Nyquist frequency* and without any significant aliasing down into the Nyquist interval! That would not be possible for evenly spaced data. It is possible here because the randomly spaced data has *some* points spaced much closer than

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the "average" sampling rate, and these remove ambiguity from any aliasing.

Implementation of the normalized periodogram in code is straightforward, with, however, a few points to be kept in mind. We are dealing with a *slow* algorithm. Typically, for N data points, we may wish to examine on the order of 2N or 4N frequencies. Each combination of frequency and data point has, in equations (13.8.4) and (13.8.5), not just a few adds or multiplies, but four calls to trigonometric functions; the operations count can easily reach several hundred times N^2 . It is highly desirable — in fact results in a factor 4 speedup — to replace these trigonometric calls by recurrences. That is possible only if the sequence of frequencies examined is a linear sequence. Since such a sequence is probably what most users would want anyway, we have built this into the implementation.

At the end of this section we describe a way to evaluate equations (13.8.4) and (13.8.5) — approximately, but to any desired degree of approximation — by a fast method [6] whose operation count goes only as $N \log N$. This faster method should be used for long data sets.

The lowest independent frequency f to be examined is the inverse of the span of the input data, $\max_i(t_i) - \min_i(t_i) \equiv T$. This is the frequency such that the data can include one complete cycle. In subtracting off the data's mean, equation (13.8.4) already assumed that you are not interested in the data's zero-frequency piece — which is just that mean value. In an FFT method, higher independent frequencies would be integer multiples of 1/T. Because we are interested in the statistical significance of any peak that may occur, however, we had better (over-) sample more finely than at interval 1/T, so that sample points lie close to the top of any peak. Thus, the accompanying program includes an oversampling parameter, called of ac; a value of ac $\gtrsim 4$ might be typical in use. We also want to specify how high in frequency to go, say f_{hi} . One guide to choosing f_{hi} is to compare it with the Nyquist frequency f_c which would obtain if the N data points were evenly spaced over the same span T, that is $f_c = N/(2T)$. The accompanying program includes an input parameter hif ac, defined as f_{hi}/f_c . The number of different frequencies N_P returned by the program is then given by

$$N_P = \frac{\text{ofac} \times \text{hifac}}{2} N \tag{13.8.9}$$

(You have to remember to dimension the output arrays to at least this size.)

The code does the trigonometric recurrences in double precision and embodies a few tricks with trigonometric identities, to decrease roundoff errors. If you are an aficionado of such things you can puzzle it out. A final detail is that equation (13.8.7) will fail because of roundoff error if z is too large; but equation (13.8.8) is fine in this regime.

SUBROUTINE period(x,y,n,ofac,hifac,px,py,np,nout,jmax,prob)
INTEGER jmax,n,nout,np,NMAX
REAL hifac,ofac,prob,px(np),py(np),x(n),y(n)
PARAMETER (NMAX=2000) Maximum expected value of n.
USES avevar
Given n data points with abscissas x(1:n) (which need not be equally spaced) and ordinates
y(1:n), and given a desired oversampling factor ofac (a typical value being 4 or larger),
this routine fills array px with an increasing sequence of frequencies (not angular frequencies)
up to hifac times the "average" Nyquist frequency, and fills array py with the values of
the Lomb normalized periodogram at those frequencies. The arrays x and y are not altered.
np, the dimension of px and py, must be large enough to contain the output, or an error
(pause) results. The routine also returns jmax such that py(jmax) is the maximum element
in py, and prob, an estimate of the significance of that maximum against the hypothesis of
random noise. A small value of prob indicates that a significant periodic signal is present.

INTEGER i,j

C

REAL ave,c,cc,cwtau,effm,expy,pnow,pymax,s,ss,sumc,sumcy,

sums,sumsh,sumsy,swtau,var,wtau,xave,xdif,xmax,xmin,yy
DOUBLE PRECISION arg,wtemp,wi(NMAX),wpi(NMAX),
 wpr(NMAX),wr(NMAX),TWOPID
PARAMETER (TWOPID=6.2831853071795865D0)
nout=0.5*ofac*hifac*n
if(nout.gt.np) pause 'output arrays too short in period'
call avevar(y,n,ave,var) Get mean and variance of the input data.
xmax=x(1)
xmin=x(1) Go through data to get the range of abscissas.

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```
do 11 j=1,n
    if(x(j).gt.xmax)xmax=x(j)
    if(x(j).lt.xmin)xmin=x(j)
enddo 11
xdif=xmax-xmin
xave=0.5*(xmax+xmin)
pymax=0.
pnow=1./(xdif*ofac)
                                         Starting frequency.
                                         Initialize values for the trigonometric recurrences
do 12 j=1,n
                                             at each data point. The recurrences are done
    arg=TWOPID*((x(j)-xave)*pnow)
    wpr(j)=-2.d0*sin(0.5d0*arg)**2
                                             in double precision.
   wpi(j)=sin(arg)
    wr(j)=cos(arg)
    wi(j)=wpi(j)
enddo 12
do 15 i=1,nout
                              Main loop over the frequencies to be evaluated.
   px(i)=pnow
    sumsh=0.
                              First, loop over the data to get \tau and related quantities.
    sumc=0.
    do 13 j=1,n
        c=wr(j)
        s=wi(j)
        sumsh=sumsh+s*c
        sumc=sumc+(c-s)*(c+s)
    enddo 13
    wtau=0.5*atan2(2.*sumsh,sumc)
    swtau=sin(wtau)
    cwtau=cos(wtau)
    sums=0.
    sumc=0.
                              Then, loop over the data again to get the periodogram value.
    sumsy=0.
    sumcy=0.
    do 14 j=1,n
        s=wi(j)
        c=wr(j)
        ss=s*cwtau-c*swtau
        cc=c*cwtau+s*swtau
        sums=sums+ss**2
        sumc=sumc+cc**2
        yy=y(j)-ave
        sumsy=sumsy+yy*ss
        sumcy=sumcy+yy*cc
        wtemp=wr(j)
                              Update the trigonometric recurrences.
        wr(j)=(wr(j)*wpr(j)-wi(j)*wpi(j))+wr(j)
        wi(j)=(wi(j)*wpr(j)+wtemp*wpi(j))+wi(j)
    enddo 14
    py(i)=0.5*(sumcy**2/sumc+sumsy**2/sums)/var
    if (py(i).ge.pymax) then
        pymax=py(i)
        imax=i
    endif
   pnow=pnow+1./(ofac*xdif) The next frequency.
enddo 15
expy=exp(-pymax)
                              Evaluate statistical significance of the maximum.
effm=2.*nout/ofac
prob=effm*expy
if(prob.gt.0.01)prob=1.-(1.-expy)**effm
return
END
```

Fast Computation of the Lomb Periodogram

We here show how equations (13.8.4) and (13.8.5) can be calculated — approximately, but to any desired precision — with an operation count only of order $N_P \log N_P$. The method uses the FFT, but it is in no sense an FFT periodogram of the data. It is an actual evaluation of equations (13.8.4) and (13.8.5), the Lomb normalized periodogram, with exactly that method's strengths and weaknesses. This fast algorithm, due to Press and Rybicki [6], makes feasible the application of the Lomb method to data sets at least as large as 10^6 points; it is already faster than straightforward evaluation of equations (13.8.4) and (13.8.5) for data sets as small as 60 or 100 points.

Notice that the trigonometric sums that occur in equations (13.8.5) and (13.8.4) can be reduced to four simpler sums. If we define

$$S_{h} \equiv \sum_{j=1}^{N} (h_{j} - \bar{h}) \sin(\omega t_{j}) \qquad C_{h} \equiv \sum_{j=1}^{N} (h_{j} - \bar{h}) \cos(\omega t_{j})$$
(13.8.10)

and

$$S_2 \equiv \sum_{j=1}^{N} \sin(2\omega t_j) \qquad C_2 \equiv \sum_{j=1}^{N} \cos(2\omega t_j)$$
(13.8.11)

then

$$\sum_{j=1}^{N} (h_j - \bar{h}) \cos \omega (t_j - \tau) = C_h \cos \omega \tau + S_h \sin \omega \tau$$

$$\sum_{j=1}^{N} (h_j - \bar{h}) \sin \omega (t_j - \tau) = S_h \cos \omega \tau - C_h \sin \omega \tau$$

$$\sum_{j=1}^{N} \cos^2 \omega (t_j - \tau) = \frac{N}{2} + \frac{1}{2} C_2 \cos(2\omega\tau) + \frac{1}{2} S_2 \sin(2\omega\tau)$$

$$\sum_{j=1}^{N} \sin^2 \omega (t_j - \tau) = \frac{N}{2} - \frac{1}{2} C_2 \cos(2\omega\tau) - \frac{1}{2} S_2 \sin(2\omega\tau)$$
(13.8.12)

Now notice that *if* the t_j s were evenly spaced, then the four quantities S_h , C_h , S_2 , and C_2 could be evaluated by two complex FFTs, and the results could then be substituted back through equation (13.8.12) to evaluate equations (13.8.5) and (13.8.4). The problem is therefore only to evaluate equations (13.8.10) and (13.8.11) for unevenly spaced data.

Interpolation, or rather reverse interpolation — we will here call it *extirpolation* — provides the key. Interpolation, as classically understood, uses several function values on a regular mesh to construct an accurate approximation at an arbitrary point. Extirpolation, just the opposite, *replaces* a function value at an arbitrary point by several function values on a regular mesh, doing this in such a way that sums over the mesh are an accurate approximation to sums over the original arbitrary point.

It is not hard to see that the weight functions for extirpolation are identical to those for interpolation. Suppose that the function h(t) to be extirpolated is known only at the discrete (unevenly spaced) points $h(t_i) \equiv h_i$, and that the function g(t) (which will be, e.g., $\cos \omega t$) can be evaluated anywhere. Let \hat{t}_k be a sequence of evenly spaced points on a regular mesh. Then Lagrange interpolation (§3.1) gives an approximation of the form

$$g(t) \approx \sum_{k} w_k(t) g(\hat{t}_k) \tag{13.8.13}$$

where $w_k(t)$ are interpolation weights. Now let us evaluate a sum of interest by the following scheme:

$$\sum_{j=1}^{N} h_j g(t_j) \approx \sum_{j=1}^{N} h_j \left[\sum_k w_k(t_j) g(\hat{t}_k) \right] = \sum_k \left[\sum_{j=1}^{N} h_j w_k(t_j) \right] g(\hat{t}_k) \equiv \sum_k \hat{h}_k g(\hat{t}_k)$$
(13.8.14)

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The general outline of the fast evaluation method is therefore this: (i) Choose a mesh size large enough to accommodate some desired oversampling factor, and large enough to have several extirpolation points per half-wavelength of the highest frequency of interest. (ii) Extirpolate the values h_i onto the mesh and take the FFT; this gives S_h and C_h in equation (13.8.10). (iii) Extirpolate the constant values 1 onto another mesh, and take its FFT; this, with some manipulation, gives S_2 and C_2 in equation (13.8.11). (iv) Evaluate equations (13.8.12), (13.8.5), and (13.8.4), in that order.

There are several other tricks involved in implementing this algorithm efficiently. You can figure most out from the code, but we will mention the following points: (a) A nice way to get transform values at frequencies 2ω instead of ω is to stretch the time-domain data by a factor 2, and then wrap it to double-cover the original length. (This trick goes back to Tukey.) In the program, this appears as a modulo function. (b) Trigonometric identities are used to get from the left-hand side of equation (13.8.5) to the various needed trigonometric functions of $\omega\tau$. FORTRAN identifiers like (e.g.) cwt and hs2wt represent quantities like (e.g.) cos $\omega\tau$ and $\frac{1}{2}\sin(2\omega\tau)$. (c) The subroutine spread does extirpolation onto the M most nearly centered mesh points around an arbitrary point; its turgid code evaluates coefficients of the Lagrange interpolating polynomials, in an efficient manner.

```
SUBROUTINE fasper(x,y,n,ofac,hifac,wk1,wk2,nwk,nout,jmax,prob)
    INTEGER jmax,n,nout,nwk,MACC
    REAL hifac,ofac,prob,wk1(nwk),wk2(nwk),x(n),y(n)
                                   Number of interpolation points per 1/4 cycle of highest fre-
    PARAMETER (MACC=4)
    USES avevar, realft, spread
                                           auency.
       Given n data points with abscissas \mathbf{x} (which need not be equally spaced) and ordinates \mathbf{y},
       and given a desired oversampling factor ofac (a typical value being 4 or larger), this routine
       fills array wk1 with a sequence of nout increasing frequencies (not angular frequencies) up
       to hifac times the "average" Nyquist frequency, and fills array wk2 with the values of the
       Lomb normalized periodogram at those frequencies. The arrays x and y are not altered.
       nwk, the dimension of wk1 and wk2, must be large enough for intermediate work space,
       or an error (pause) results. The routine also returns jmax such that wk2(jmax) is the
       maximum element in wk2, and prob, an estimate of the significance of that maximum
       against the hypothesis of random noise. A small value of prob indicates that a significant
       periodic signal is present.
    INTEGER j,k,ndim,nfreq,nfreqt
    REAL ave, ck, ckk, cterm, cwt, den, df, effm, expy, fac, fndim, hc2wt,
         hs2wt, hypo, pmax, sterm, swt, var, xdif, xmax, xmin
    EXTERNAL spread
    nout=0.5*ofac*hifac*n
   nfreqt=ofac*hifac*n*MACC
                                   Size the FFT as next power of 2 above nfreqt.
    nfreq=64
    if (nfreq.lt.nfreqt) then
1
        nfreq=nfreq*2
    goto 1
    endif
    ndim=2*nfreq
    if(ndim.gt.nwk) pause 'workspaces too small in fasper'
    call avevar(y,n,ave,var)
                                   Compute the mean, variance, and range of the data.
    xmin=x(1)
    xmax=xmin
    do 11 j=2,n
        if(x(j).lt.xmin)xmin=x(j)
        if(x(j).gt.xmax)xmax=x(j)
    enddo 11
    xdif=xmax-xmin
    do 12 j=1,ndim
                                   Zero the workspaces
        wk1(i)=0.
        wk2(j)=0.
    enddo 12
```

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```
fac=ndim/(xdif*ofac)
fndim=ndim
                              Extirpolate the data into the workspaces.
do 13 j=1,n
   ck=1.+mod((x(j)-xmin)*fac,fndim)
   ckk=1.+mod(2.*(ck-1.),fndim)
   call spread(y(j)-ave,wk1,ndim,ck,MACC)
   call spread(1.,wk2,ndim,ckk,MACC)
enddo 13
call realft(wk1,ndim,1)
                              Take the Fast Fourier Transforms.
call realft(wk2.ndim.1)
df=1./(xdif*ofac)
k=3
pmax=-1.
                              Compute the Lomb value for each frequency.
do 14 j=1,nout
   hypo=sqrt(wk2(k)**2+wk2(k+1)**2)
   hc2wt=0.5*wk2(k)/hypo
   hs2wt=0.5*wk2(k+1)/hypo
   cwt=sqrt(0.5+hc2wt)
   swt=sign(sqrt(0.5-hc2wt),hs2wt)
   den=0.5*n+hc2wt*wk2(k)+hs2wt*wk2(k+1)
   cterm=(cwt*wk1(k)+swt*wk1(k+1))**2/den
   sterm=(cwt*wk1(k+1)-swt*wk1(k))**2/(n-den)
   wk1(j)=j*df
    wk2(j)=(cterm+sterm)/(2.*var)
    if (wk2(j).gt.pmax) then
        pmax=wk2(j)
        jmax=j
    endif
   k=k+2
enddo 14
                              Estimate significance of largest peak value.
expy=exp(-pmax)
effm=2.*nout/ofac
prob=effm*expy
if(prob.gt.0.01)prob=1.-(1.-expy)**effm
return
END
SUBROUTINE spread(y,yy,n,x,m)
INTEGER m,n
REAL x,y,yy(n)
   Given an array yy of length n, extirpolate (spread) a value y into m actual array elements
   that best approximate the "fictional" (i.e., possibly noninteger) array element number \boldsymbol{x}.
   The weights used are coefficients of the Lagrange interpolating polynomial.
INTEGER ihi,ilo,ix,j,nden,nfac(10)
REAL fac
SAVE nfac
DATA nfac /1,1,2,6,24,120,720,5040,40320,362880/
if(m.gt.10) pause 'factorial table too small in spread'
ix=x
if(x.eq.float(ix))then
   yy(ix)=yy(ix)+y
else
   ilo=min(max(int(x-0.5*m+1.0),1),n-m+1)
   ihi=ilo+m-1
   nden=nfac(m)
   fac=x-ilo
   do n j=ilo+1,ihi
       fac=fac*(x-j)
    enddo 11
   yy(ihi)=yy(ihi)+y*fac/(nden*(x-ihi))
   do 12 j=ihi-1,ilo,-1
       nden=(nden/(j+1-ilo))*(j-ihi)
```

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13.9 Computing Fourier Integrals Using the FFT

Not uncommonly, one wants to calculate accurate numerical values for integrals of the form

$$I = \int_{a}^{b} e^{i\omega t} h(t) dt , \qquad (13.9.1)$$

or the equivalent real and imaginary parts

$$I_c = \int_a^b \cos(\omega t) h(t) dt \qquad I_s = \int_a^b \sin(\omega t) h(t) dt , \qquad (13.9.2)$$

and one wants to evaluate this integral for many different values of ω . In cases of interest, h(t) is often a smooth function, but it is not necessarily periodic in [a, b], nor does it necessarily go to zero at a or b. While it seems intuitively obvious that the *force majeure* of the FFT ought to be applicable to this problem, doing so turns out to be a surprisingly subtle matter, as we will now see.

Let us first approach the problem naively, to see where the difficulty lies. Divide the interval [a, b] into M subintervals, where M is a large integer, and define

$$\Delta \equiv \frac{b-a}{M}, \quad t_j \equiv a+j\Delta, \quad h_j \equiv h(t_j), \quad j = 0, \dots, M$$
(13.9.3)

Notice that $h_0 = h(a)$ and $h_M = h(b)$, and that there are M + 1 values h_j . We can approximate the integral I by a sum,

$$I \approx \Delta \sum_{j=0}^{M-1} h_j \exp(i\omega t_j)$$
(13.9.4)

which is at any rate first-order accurate. (If we centered the h_j 's and the t_j 's in the intervals, we could be accurate to second order.) Now for certain values of ω and M, the sum in equation (13.9.4) can be made into a discrete Fourier transform, or DFT, and evaluated by the fast Fourier transform (FFT) algorithm. In particular, we can choose M to be an integer power of 2, and define a set of special ω 's by

$$\omega_m \Delta \equiv \frac{2\pi m}{M} \tag{13.9.5}$$

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