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FAST ALGORITHM FOR SPECTRAL ANALYSIS OF UNEVENLY SAMPLED DATA

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ABSTRACT

The Lomb-Scargle method performs spectral analysis on unevenly sampled data and is known to be a powerful way to find, and test the significance of, weak periodic signals. The method has previously been thought to be "slow," requiring of order 10^2N^2 operations to analyze N data points. We show that Fast Fourier Transforms (FFTs) can be used in a novel way to make the computation of order $10^2N \log N$. Despite its use of the FFT, the algorithm is in no way equivalent to conventional FFT periodogram analysis.
Subject heading: numerical methods

I. INTRODUCTION

Lomb (1976) and Scargle (1982) developed a novel type of periodogram (Fourier spectrum) analysis, quite powerful for finding, and testing the significance of, weak periodic signals in otherwise random, *unevenly sampled* data. Horne and Baliunas (1986) have elaborated on the method and discussed its implementation. The method is incorporated into the data analysis package " J " and is widely used in some astronomical specialities. (For a pedagogical discussion, see Press and Teukolsky 1989).

Briefly, given a set of data values h_i, $i = 1, \ldots, N$ at respective observation times t_i, the Lomb-Scargle periodogram is constructed as follows. First, compute the data's mean and variance by

$$\bar{h} \equiv \frac{1}{N}\sum_1^N h_i\,, \qquad \sigma^2 \equiv \frac{1}{N-1}\sum_1^N (h_i - \bar{h})^2 \tag{1}$$

Second, for each angular frequency $\omega \equiv 2\pi f > 0$ of interest, compute a time-offset τ by

$$\tan(2\omega\tau) = \frac{\sum_j \sin 2\omega t_j}{\sum_j \cos 2\omega t_j} \tag{2}$$

Third, the Lomb-Scargle *normalized periodogram* (spectral power as a function of ω) is defined by

$$P_N(\omega) \equiv \frac{1}{2\sigma^2}\left\{\frac{[\sum_j (h_j - \bar{h})\cos\omega(t_j-\tau)]^2}{\sum_j \cos^2\omega(t_j-\tau)} + \frac{[\sum_j (h_j - \bar{h})\sin\omega(t_j-\tau)]^2}{\sum_j \sin^2\omega(t_j-\tau)}\right\} \tag{3}$$

The constant τ makes $P_N(\omega)$ completely independent of shifting all the t_i's by any constant. Lomb (1976) showed that this particular choice of offset has another, deeper, effect: it makes equation (3) 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

$$h(t) = A\cos\omega t + B\sin\omega t\,. \tag{4}$$

This fact gives some insight into why the method gives superior results on unevenly sampled data: it weights the data on a "per point" basis instead of on a "per time interval" basis.

Up to now, the Lomb-Scargle method has been viewed as being a "slow" method, in the technical sense of requiring a number of operations on the order of $N_\omega N$ operations to examine N_ω frequencies for a data set of N points. In fact, the constant in front of this order is quite large, $\sim 10^2$, because of the trigonometric operations which are required. Restriction to evenly spaced values of ω and use of trigonometric recurrence relations (Press and Teukolsky 1988) can save a factor ~ 3, but the count is still large.

Furthermore, one typically wants N_ω to be larger than N by a significant factor, for two independent reasons. First, it is desirable to oversample the spectrum, so as not to miss the peak of a spectral signal that is on the borderline of statistical significance. Second—this is one of the powerful features of the method—it is often meaningful to examine frequencies significantly higher than the Nyquist frequency that would obtain if the same number of data points were evenly spaced in the same total length of time. Some spectral information is obtainable for frequencies all the way up to something like half the inverse spacing of the *closest* spaced points.

The upshot is that the Lomb-Scargle method has a computational burden on the order of N^2, with quite a large constant in front, $\sim 10^2$–10^3. Until now, its use has been limited to data sets no longer than, say, 1000 points for interactive workstation applications, or perhaps 10^4 points on a supercomputer.

In the remainder of this paper, we will show how equations (2) and (3) can be calculated—approximately, but to any desired precision—with an operation count only of order $N_\omega \log N_\omega$. The method uses the FFT, but it is in no sense an FFT periodogram of the data. It is an actual evaluation of equations (2) and (3), the Lomb-Scargle normalized periodogram, with exactly that method's strengths and weaknesses. The fast algorithm given here makes feasible the application of the Lomb-Scargle method to data sets at least as large as 10^6 points, and it is already faster than straightforward evaluation of equations (2) and (3) for data sets as small as 60 or 100 points.

II. FAST LOMB-SCARGLE EVALUATION

A first observation to be made is that the trigonometric sums that occur in equations (2) and (3) can be reduced to four simpler sums. If we define

$$S_h \equiv \sum_{j=1}^{N} h_j \sin(\omega t_j), \qquad C_h \equiv \sum_{j=1}^{N} h_j \cos(\omega t_j) \tag{5}$$

and

$$S_2 \equiv \sum_{j=1}^{N} \sin(2\omega t_j) \qquad C_2 \equiv \sum_{j=1}^{N} \cos(2\omega t_j), \tag{6}$$

then

$$\begin{aligned}
&\sum_{j=1}^{N} h_j \cos \omega(t_j - \tau) = C_h \cos \omega\tau + S_h \sin \omega\tau \\
&\sum_{j=1}^{N} h_j \sin \omega(t_j - \tau) = S_h \cos \omega\tau - C_h \sin \omega\tau \\
&\sum_{j=1}^{N} \cos^2 \omega(t_j - \tau) = \frac{N}{2} + \frac{1}{2} C_2 \cos(2\omega\tau) + \frac{1}{2} S_2 \sin(2\omega\tau) \\
&\sum_{j=1}^{N} \sin^2 \omega(t_j - \tau) = \frac{N}{2} - \frac{1}{2} C_2 \cos(2\omega\tau) - \frac{1}{2} S_2 \sin(2\omega\tau)
\end{aligned} \tag{7}$$

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 (7) to evaluate equations (2) and (3). The problem is therefore only to evaluate equations (5) and (6) for unevenly spaced data.

Interpolation, or rather "reverse interpolation"—hereafter referred to as "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 (see, e.g., Press *et al.* 1986, § 3.1) gives an approximation of the form

$$g(t) \approx \sum_k w_k(t) g(\hat{t}_k), \tag{8}$$

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

$$\sum_{j=1}^{N} h_j g(t_j) \approx \sum_{j=1}^{N} h_j \left[\sum_k w_k(t_j) g(\hat{t}_k)\right] = \sum_k \left[\sum_{j=1}^{N} h_j w_k(t_j)\right] g(\hat{t}_k) \equiv \sum_k \hat{h}_k g(\hat{t}_k). \tag{9}$$

Here $\hat{h}_k \equiv \sum_j h_j \omega_k(t_j)$. Notice that equation (9) replaces the original sum by one on the regular mesh. Notice also that the accuracy of equation (8) depends only on the fineness of the mesh with respect to the function g and has nothing to do with the spacing of the points t_j or the function h; therefore the accuracy of equation (9) also has this property.

The general outline of the fast evaluation method is therefore this: (1) 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. (2) Extirpolate the values h_i onto the mesh and take the FFT; this gives S_h and C_h in equation (5). (3) Extirpolate the constant values 1 onto another mesh, and take its FFT; this, with some manipulation, gives S_2 and C_2 in equation (6). (4) Evaluate equations (7) (2), and (3), in that order.

There are several other tricks involved in implementing this algorithm efficiently. Rather than try to describe these in words, we direct attention to the commented program implementation, reproduced in Table 1, mentioning here only 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 of 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*) The subroutine REALFT is assumed to return the positive-frequency half of the complex spectrum of a real data array, and can be found in Press *et al.* (1986). (*c*) Trigonometric identities are used to get from the left-hand side of equation (2) 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 $\frac{1}{2} \sin(2\omega\tau)$. (*d*) See Press and Teukolsky (1988) for discussion of the approximations involved in the calculation of the significance level of the largest spectral peak found. (*e*) 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, as efficiently as we know how to do.

TABLE 1

FORTRAN SUBROUTINE FOR FAST EVALUATION OF THE LOMB-SCARGLE STATISTIC

```
  SUBROUTINE FASPER(X,Y,N,OFAC,HIFAC,WK1,WK2,NWK,NOUT,JMAX,PROB)
    Given N data points with abscissas X (which need not be equally spaced) and ordinates 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-Scargle 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 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.
  PARAMETER (MACC=4)                  Number of interpolation points per 1/4 cycle of highest
  REAL X(N),Y(N),WK1(NWK),WK2(NWK)        frequency.
  NOUT=0.5*OFAC*HIFAC*N
  NFREQT=OFAC*HIFAC*N*MACC            Size the FFT as next power of 2 above NFREQT.
  NFREQ=64
1 IF (NFREQ.LT.NFREQT) THEN
    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)
  11 CONTINUE
  XDIF=XMAX-XMIN
  DO 12 J=1,NDIM                      Zero the workspaces.
    WK1(J)=0.
    WK2(J)=0.
  12 CONTINUE
  FAC=NDIM/(XDIF*OFAC)
  FNDIM=NDIM
  DO 13 J=1,N                         Extirpolate the data into the workspaces.
    CK=1.+AMOD((X(J)-XMIN)*FAC,FNDIM)
    CKK=1.+AMOD(2.*(CK-1.),FNDIM)
    CALL SPREAD(Y(J)-AVE,WK1,NDIM,CK,MACC)
    CALL SPREAD(1.,WK2,NDIM,CKK,MACC)
  13 CONTINUE
  CALL REALFT(WK1,NFREQ,1)            Take the Fast Fourier Transforms.
  CALL REALFT(WK2,NFREQ,1)
  DF=1./(XDIF*OFAC)
  K=3
  PMAX=-1.
  DO 14 J=1,NOUT                      Compute the Lomb-Scargle value for each frequency.
    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
  14 CONTINUE                         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)
    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 non-integer) array element number X.
    The weights used are coefficients of the Lagrange interpolating polynomial.
  REAL YY(N), NFAC(10) /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 15 J=ILO+1,IHI
      FAC=FAC*(X-J)
    15 CONTINUE
    YY(IHI)=YY(IHI)+Y*FAC/(NDEN*(X-IHI))
    DO 16 J=IHI-1,ILO,-1
      NDEN=(NDEN/(J+1-ILO))*(J-IHI)
      YY(J)=YY(J)+Y*FAC/(NDEN*(X-J))
    16 CONTINUE
  ENDIF
  RETURN
  END
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