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A PRESCRIPTION FOR PERIOD ANALYSIS OF UNEVENLY SAMPLED TIME SERIES

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ABSTRACT

We present a technique for detecting the presence and significance of a period in unequally sampled time series data. We review the calculation of the modified periodogram for unevenly sampled data. We clarify the proper definition of the variance that is used to normalize the power of the modified periodogram. We prove that the probability that a peak in the periodogram is noise or signal can be easily assessed by the method given here only when the *total* variance of the data is used to normalize the periodogram power.

We discuss the crucial choice of independent frequencies in calculating both the periodogram and the false alarm probability from unevenly sampled data. We derive an empirical formula for estimating the number of independent frequencies.

In addition, we review the formula for the uncertainty of a frequency identified in the periodogram. We prescribe a method for detecting the presence of an alias frequency caused by the interaction of the window and signal.

With some examples of periodic signals, we show the minimum number of points required to measure reliably a signal. We investigate the signal-to-noise ratio and the number of points required to extract signals when one or two periodicities are present in the time series.

Subject headings: numerical methods

I. INTRODUCTION

Many astronomical processes are periodic in nature, and the best known way to describe these periodicities is through Fourier analysis. Because of the nature of observational astronomy, the data to be analyzed are frequently unevenly spaced in time and often contain large amounts of random (and even nonrandom) noise. Rebinning the unevenly sampled data to equally spaced bins and calculating a conventional periodogram may alter the perceived frequency and significance of a periodic signal.

In this paper we discuss the normalized periodogram given by Scargle (1982), whose method treats without bias the periodogram calculated for unevenly sampled time series. Scargle (1982) also provides, through the "false alarm probability," a simple estimate of the significance of the height of a peak in the power spectrum. A debate has arisen concerning the correct normalization of the periodogram required to achieve the simple exponential probability distribution that Scargle (1982) derives (Black and Scargle 1982; Lockwood *et al.* 1984; Baliunas *et al.* 1985; Brosius, Mullan, and Stencel 1985; Gilliland and Fisher 1985). Scargle (1982) normalizes the periodogram by σ^2, the variance of the noise. Some people have incorrectly interpreted the phrase "variance of the noise" to mean the variance remaining after a sine curve has been removed from the data, or to mean the observational uncertainty. We prove that these interpretations of the variance destroy the exponential behavior of the probability distribution of the periodogram and invalidate the subsequent estimates of the false alarm probability. The probability that a given frequency is a true signal can be estimated correctly only when the periodogram power is normalized by the *total* variance of the data.

Upon further analysis of the modified periodogram, we discover some important properties concerning the number of independent frequencies. With simulated sets of data and periodograms of these data, we derive an empirical formula that estimates the correct number of independent frequencies to use when calculating the false alarm probability.

We also examine the impact of signal-to-noise ratio, number of sampled points, aliasing, and multiple signal frequencies on the calculated periodogram. We provide an estimate of the error in frequency of a significant peak in a periodogram. These techniques should be valuable for analyzing a wide variety of time series measurements.

II. CALCULATING THE PERIODOGRAM

For a times series $X(t_i)$, where $i = 1, 2, \ldots, N_0$, the periodogram as a function of the frequency ω is defined (Scargle 1982) as

$$P_X(\omega) = \frac{1}{2}\left\{\frac{[\sum_{j=1}^{N_0} X(t_j)\cos\omega(t_j-\tau)]^2}{\sum_{j=1}^{N_0}\cos^2\omega(t_j-\tau)} + \frac{[\sum_{j=1}^{N_0} X(t_j)\sin\omega(t_j-\tau)]^2}{\sum_{j=1}^{N_0}\sin^2\omega(t_j-\tau)}\right\}, \quad (1)$$

where τ is defined by the equation

$$\tan(2\omega\tau) = \left(\sum_{j=1}^{N_0}\sin 2\omega t_j\right)\Big/\left(\sum_{j=1}^{N_0}\cos 2\omega t_j\right). \quad (2)$$

When $P_X(\omega)$ is defined in this manner, it has several useful properties which the usual discrete Fourier transform does not have. First, the inclusion of the τ terms makes the periodogram invariant to a shift of the origin of time. Second, this form makes periodogram analysis exactly equivalent to least-squares fitting of sine curves to the data. More importantly, $P_X(\omega)$ is defined so that if the signal $X(t_j)$ is purely noise, then the power in $P_X(\omega)$ follows an exponential probability distribution. This exponential distribution provides a convenient estimate of the probability that a given peak is a true signal, or whether it is the result of randomly distributed noise.

a) *The Correct Variance*

The correct normalization factor for $P_X(\omega)$ is the total variance of the data. The proof of this statement can be derived following a close look at Appendix A in Scargle (1982). The function $P_X(\omega)$ can be rewritten as

$$P_X(\omega) = \tfrac{1}{2}[C^2(\omega) + S^2(\omega)] , \tag{3}$$

where

$$C(\omega) = A \sum_j X(t_j) \cos \omega(t_j - \tau) , \tag{4}$$

$$S(\omega) = B \sum_j X(t_j) \sin \omega(t_j - \tau) , \tag{5}$$

$$A(\omega) = \left[\sum_j \cos^2 \omega(t_j - \tau)\right]^{-1/2} , \tag{6}$$

and

$$B(\omega) = \left[\sum_j \sin^2 \omega(t_j - \tau)\right]^{-1/2} . \tag{7}$$

Now, if we assume that X is pure independently and normally (Gaussian) distributed noise with zero mean and constant variance $\sigma_0{}^2$, then we can write its distribution function as $n(y; 0, \sigma_0{}^2) = 1/[\sigma_0(2\pi)^{1/2}]e^{-y^2/2\sigma_0{}^2}$. The function $C(\omega)$ is a linear combination of independent normally distributed random variables, so it too is a normal random variable. The mean of C is zero, $\langle C \rangle = 0$, and

$$\sigma_c{}^2 = \langle C^2 \rangle = A^2\sigma_0{}^2 \sum_j \cos^2 \omega(t_j - \tau) = \sigma_0{}^2 . \tag{8}$$

Similarly, $S(\omega)$ is a normal random variable with zero mean, $\langle S \rangle = 0$, and

$$\sigma_s{}^2 = \langle S^2 \rangle = B^2\sigma_0{}^2 \sum_j \sin^2 \omega(t_j - \tau) = \sigma_0{}^2 = \sigma_c{}^2 . \tag{9}$$

$C(\omega)$ and $S(\omega)$ are normal random variables *only* if X is also a normal random variable.

With these assumptions, it is simple to show that the distribution functions for $C^2(\omega)$ and $S^2(\omega)$ have identical gamma density functions of the form

$$\Gamma\left(x; \alpha = \frac{1}{2}, \sigma\right) = \frac{1}{\sigma(2\pi x)^{1/2}} e^{-x/2\sigma^2} . \tag{10}$$

$P_X(\omega)$ is the sum of these two functions with gamma distributions (divided by 2), so it has the distribution function (cf. Hoel, Port, and Stone 1971)

$$\Gamma(z; \alpha_c + \alpha_s = 1, \sigma) = \frac{1}{\sigma^2} e^{-z/\sigma^2} . \tag{11}$$

Thus, *only* when the periodogram is normalized by the total variance,

$$P_N(\omega) = P_X(\omega)/\sigma^2 , \tag{12}$$

does the periodogram have the desired e^{-z} probability distribution. Other distribution functions for X give different distribution functions for C and S, which consequently yield different distributions for P_N.

We would like to emphasize the importance of normalizing the periodogram by the total variance of the data and not by an estimate of the noise derived either from the residuals after a signal has been removed or from the uncertainty in the measurement. There are two reasons why any estimate other than the total variance is unacceptable in the normalization. First, the subtraction of a sinusoid from the data assumes a signal is present. In this case, the subsequent use of the false alarm probability to test for the presence of the same signal is circular reasoning and therefore fallacious. More importantly, it is *only* the normalization by the total variance of the data that yields the correct statistical behavior of the periodogram. Other normalizations will not produce the desired exponential distributions.

b) *The False Alarm Probability, F*

The e^{-z} distribution is very useful, because it means that for any frequency ω_0, the probability that $P_N(\omega_0)$ is of height z or higher is Pr $[P_N(\omega_0) > z] = e^{-z}$. Suppose that z is the highest peak in a periodogram that sampled N_i independent frequencies. The probability that each independent frequency is smaller than z is $1 - e^{-z}$ so the probability that every frequency is lower than z is $[1 - e^{-z}]^{N_i}$. Thus, the probability that some peak is of height z or higher is the false alarm probability $F = 1 - [1 - e^{-z}]^{N_i}$ (cf. Scargle 1982). The false alarm probability tells us the probability that a peak of height z or hither will occur, *assuming that the data are pure noise.* Consequently, the quantity $1 - F$ is the probability that the data contain a signal. It is vitally important, however, that we define the normalized periodogram $P_N(\omega) = P_X(\omega)/\sigma^2$, where σ^2 is the *total* variance of the data. Any other normalization except the total variance of the data will destroy the definition of the false alarm probability given above. It is therefore unjustified to use any other value for σ^2, such as an independent estimate of the experimental error or the variance after a sine curve has been subtracted.

c) The Number of Independent Frequencies

An important ingredient for the calculation of the false alarm probability is the number of independent frequencies, N_i. To determine the correct value of N_i, we simulated a large number of data sets. All data sets were pseudo-Gaussian noise, with several different spacings in the time coordinate. There were three major types of simulations. First, the data were evenly spaced in time. Second, each time followed the previous time by a random number between 0 and 1. Third, data were clumped in groups of three points at each evenly spaced time interval. The periodogram of each data set was evaluated from $\omega = 2\pi/T$ to $\omega = \pi N_0/T$, where T is the total time interval. The periodogram frequencies range from a single frequency up to the Nyquist frequency, so they include all of the periods that can be safely studied in each time series. The highest peak then was chosen in each periodogram. The highest peaks from periodograms were then combined, and a false alarm function $1 - [1 - e^{-z}]^{N_i}$ was fitted to the peak distribution with N_i as the variable parameter. The results of the simulations are shown in Table 1. We fitted a parabola to the empirically generated values of N_i as a function of N_0 and derived the formula

$$N_i = -6.362 + 1.193N_0 + 0.00098N_0^2 . \tag{13}$$

With unevenly spaced data, the power in the sidelobes of the peaks of the window function is greatly reduced (Deeming 1975). The reduction in power in turn suppresses the possible combinations of frequencies that lead to peaks. Therefore, deviations from the evenly spaced case can actually reduce the number of independent frequencies, for example, down to $N_i = N_0/2.9$ in the case of three data points clumped per time point (see Table 1). Not surprisingly, simply evaluating unevenly sampled data may be preferable to rebinning it into equally spaced bins. The rebinned data will have more independent frequencies and a less significant false alarm probability than the unevenly sampled data.

d) Spectral Leakage

Occasionally more than one peak with a significant height according to the false alarm probability appears in a periodogram. Multiple, significant peaks may be caused by the presence of more than one periodic signal in the data. Alternatively, a true signal at frequency ω_0 can cause peaks in the periodogram at frequencies other than ω_0 because of the finite length of the data window and irregularities in the data spacing. These sidelobe peaks in the window function may have significant heights. This problem is commonly referred to as spectral leakage, or aliasing if power from high frequencies leaks to lower frequencies. One useful method of determining whether any additional peaks with significant false alarm probability are physically real is to subtract from the data a sine curve with frequency ω_0 corresponding to the most significant peak and then to recompute the periodogram. A good computational method for subtracting a sinusoid may be found in Ferraz-Mello (1981). This procedure lessens the problem of leakage to a great degree. After filtering, any remaining significant frequencies other than ω_0 are likely to be signals. For this second periodogram, however, the probability analysis is slightly different than that of a periodogram with no sine curve subtracted. The second periodogram has been created under the assumption that a frequency ω_0 does indeed exist in the data, and a sinusoid with that frequency has then been subtracted from the data. Therefore, the second periodogram must be normalized by the variance of

TABLE 1

INDEPENDENT FREQUENCIES IN SIMULATED DATA

Number of Data Points (N_0)	Number of Independent Frequencies (N_i)	Number of Tests	Type of Spacing
10	9.70	1395	even
15	14.45	347	even
25	27.38	213	even
35	38.40	214	even
50	54.45	369	even
64	71.76	512	even
75	86.05	153	even
100	119.58	296	even
128	152.53	913	even
170	218.33	218	even
256	369.97	224	even
300	455.95	107	even
400	618.69	106	even
128	43.90	1094	clumps of 3
128	137.34	587	random

the data *after* the sine curve with frequency ω_0 has been subtracted. Additionally, the probabilities for any frequencies determined in this manner should be quoted as the probability that the frequency is real assuming that there exists a signal at ω_0.

e) Uncertainty in the Frequency

It is also possible to compute the uncertainty in the determination of a frequency. Kovacs (1981) found the standard deviation of the frequency to be

$$\delta\omega = \frac{3\pi\sigma_N}{2(N_0)^{1/2}TA}, \tag{14}$$

where A is the amplitude of the signal, σ_N^2 is the variance of the noise after the signal has been subtracted, and T is the total length of the data set. Kovacs's derivation assumes a single signal, with Gaussian noise, and even data spacing. Uneven data spacing does not seem to degrade the uncertainty to any noticeable degree (cf. Baliunas *et al.* 1985). Multiple signals, on the other hand, can cause further shifts in detected frequencies if they are closely spaced (Kovacs 1981). Linear trends over the span of the data can also cause additional shifts in the determined frequency.

III. EXAMPLES OF PERIODOGRAM ANALYSIS

With these definitions, it is easy to calculate the sensitivity of the modified periodogram technique to a variety of signals.

a) Pure Signals

First, let us assume that our signal is a pure sine curve, so that $X(t) = X_0 \cos \omega_0 t$. In this case, $\langle X \rangle = 0$ and $\sigma_0^2 = \langle X^2 \rangle = X_0^2/2$. If we ignore the τ terms, which are usually very minor corrections and assume that the t_j are not badly bunched in time, then $\sum_j \cos^2 \omega t_j = N_0/2$ so

$$C(\omega_0) = A \sum_j X_0 \cos^2 \omega_0 t_j = X_0(N_0/2)^{1/2} \tag{15}$$

and

$$S(\omega_0) = B \sum_j X_0 \cos \omega_0 t_j \sin \omega_0 t_j = 0 \tag{16}$$

so

$$P_N(\omega_0) = C^2(\omega_0)/2\sigma_0^2 = N_0/2\ , \tag{17}$$

and

$$F = 1 - [1 - e^{-N_0/2}]^{N_i}\ . \tag{18}$$

Some values for F are tabulated in Table 2. The results listed in Table 2 show that the peaks quickly become very significant, with only twelve points needed for 95% certainty that a signal exists. The table starts with five points, because the periodogram determines four parameters: the amplitude, the frequency, the phase, and an additive constant. Thus, the modified periodogram requires sampling at least five points, and preferably many more points.

b) Signal Plus Noise

Most real data sets consist of a signal plus noise, so it is instructive to consider the case where $X(t) = X_0 \cos \omega_0 t + R(t)$, where $R(t)$ is a randomly distributed normal variable with variance σ_r^2 and zero mean. In this case, we still have $\langle X \rangle = 0$ and

$$\sigma_0^2 = \langle X^2 \rangle = (X_0^2/2) + \sigma_r^2 + X_0\langle R(t) \cos \omega_0 t \rangle = (X_0^2/2) + \sigma_r^2\ . \tag{19}$$

TABLE 2

FALSE ALARM PROBABILITIES FOR A PURE SIGNAL

False Alarm Probability	Number of Sampled Points
0.7138	5
0.5402	6
0.3845	7
0.2622	8
0.1737	9
0.1129	10
0.0724	11
0.0461	12
0.0292	13
0.0184	14
0.0116	15
0.0011	20
1×10^{-5}	30
8×10^{-8}	40
5×10^{-10}	50

Additionally,

$$C(\omega_0) = X_0(N_0/2)^{1/2} + A \sum_j R(t_j) \cos \omega_0 t_j = X_0(N_0/2)^{1/2} \tag{20}$$

and $S(\omega_0) = 0$ so

$$P_N(\omega_0) = \frac{X_0^2 N_0}{2X_0^2 + 4\sigma_r^2} = \frac{N_0}{2}\left(1 + \frac{2\sigma_r^2}{X_0^2}\right)^{-1} . \tag{21}$$

We define the signal-to-noise ratio $\xi = X_0^2/2\sigma_r^2$, which is the ratio of the power caused by the signal to the power caused by the noise. The false alarm probability is

$$F = 1 - [1 - e^{-(N_0/2)(1+\xi^{-1})^{-1}}]^{N_i} , \tag{22}$$

which can be rearranged to yield the value of ξ necessary to detect a signal with a failure rate F,

$$\xi = -\left\{1 + \frac{N_0}{2 \ln [1 - (1 - F)^{1/N_i}]}\right\}^{-1} . \tag{23}$$

Table 3 shows the necessary values of ξ to be 95% certain that a signal exists for a variety of values of N_0. The periodogram can pick out the signal even for very poor signal-to-noise ratios, as long as some modest number of points are sampled. The table also shows the uncertainty in the discovered period, $(\delta\omega)T$. This uncertainty decreases as N_0 increases, even though F stays the same. This can be understood by considering the general rule from statistics that the uncertainty of the resolution of the centroid of a peak is equal to $s/n^{1/2}$, where s is the standard deviation of the peak and n is the number of points.

To further illustrate the value of the normalized periodogram in detecting a weak signal from noisy data, we constructed a sample signal $X(t) = 0.75 \cos(0.6t) + R(t)$, where $R(t)$ is Gaussian noise with a variance $\sigma_r^2 = 0.902$. The period of this signal is 10.47 time units. We sampled this signal at the integers between 1 and 100, threw away 10 points randomly, and found that $\sigma_0^2 = 1.199$ so $\xi = 0.313$. The resultant signal is shown in Figure 1. The initial period cannot be detected by visual inspection because the signal-to-noise ratio is so poor. We then calculated the power spectrum displayed in Figure 2.

The smallest frequency we sampled, $2\pi/T$, corresponds to just one cycle in the data. This is not a firm lower limit. Clear signals with period slightly longer than T can sometimes be detected, but with poor resolution. All periods with less than two cycles in the data are somewhat questionable, as they could have been caused by an event such as a single flare. The largest frequency we calculated was $\pi N_0/T$ which is the traditional Nyquist frequency for evenly spaced data. The Nyquist frequency is not well defined for unevenly spaced signals, but it can serve as a reasonable upper limit for the calculation. We generally sample the periodogram with a coarse frequency spacing of about $1/T$. This procedure samples each peak well enough, without requiring excessive computation time. Recomputing the periodogram in the region around the highest peak with higher resolution gives more precise values of the peak height and frequency. We caution that the mean must be subtracted from the data before the periodogram is computed. A nonzero mean of the data will destroy the probability distribution and may cause other problems.

In our simulation, the highest peak is situated at $\omega = 0.608$ with a height of $z = 13.34$ (Fig. 2). The false alarm probability (eq. [18]) in this case yields $F = 1.52 \times 10^{-4}$, which means that only 1 in 6600 data sets with the same variance and no sine curve will have a peak of that height or higher. For comparison, we have marked on Figure 2 several false alarm levels. The 50% line is the level above which half of all noise spectrums will have one or more peaks when there are 90 data points. The 10% line is the level above which 10% of all noise spectrums will have one or more peaks, and so forth. The uncertainty in the frequency we calculate to be $\delta\omega = 0.006$ (eq. [14]), so $\omega = 0.608 \pm 0.006$, or almost exactly the same as the frequency we used to create the signal. Notice that it is impossible to pick this signal out by eye, but the signal is clearly detected by the periodogram.

c) Two Sinusoids Plus Noise

If our signal is the sum of two sines, then $X(t) = X_0 \cos \omega_0 t + X_1 \cos \omega_1 t + R(t)$. Once again, $\langle X \rangle = 0$ and

$$\sigma_0^2 = (X_0^2/2) + (X_1^2/2) + \sigma_r^2 + X_0 X_1 \langle \cos \omega_0 t \cos \omega_1 t \rangle = (X_0^2/2) + (X_1^2/2) + \sigma_r^2 . \tag{24}$$

TABLE 3

REQUIRED ξ FOR 5% FALSE ALARM PROBABILITY

Number of Sampled Points	Signal-to-noise Ratio (ξ)	Uncertainty in Frequency $(\delta\omega)T$
12	0.473	1.40
13	0.431	1.41
14	0.397	1.41
15	0.368	1.42
20	0.276	1.42
30	0.192	1.39
40	0.152	1.35
50	0.128	1.32
100	0.077	1.20
200	0.047	1.08
500	0.025	0.95
1000	0.015	0.87

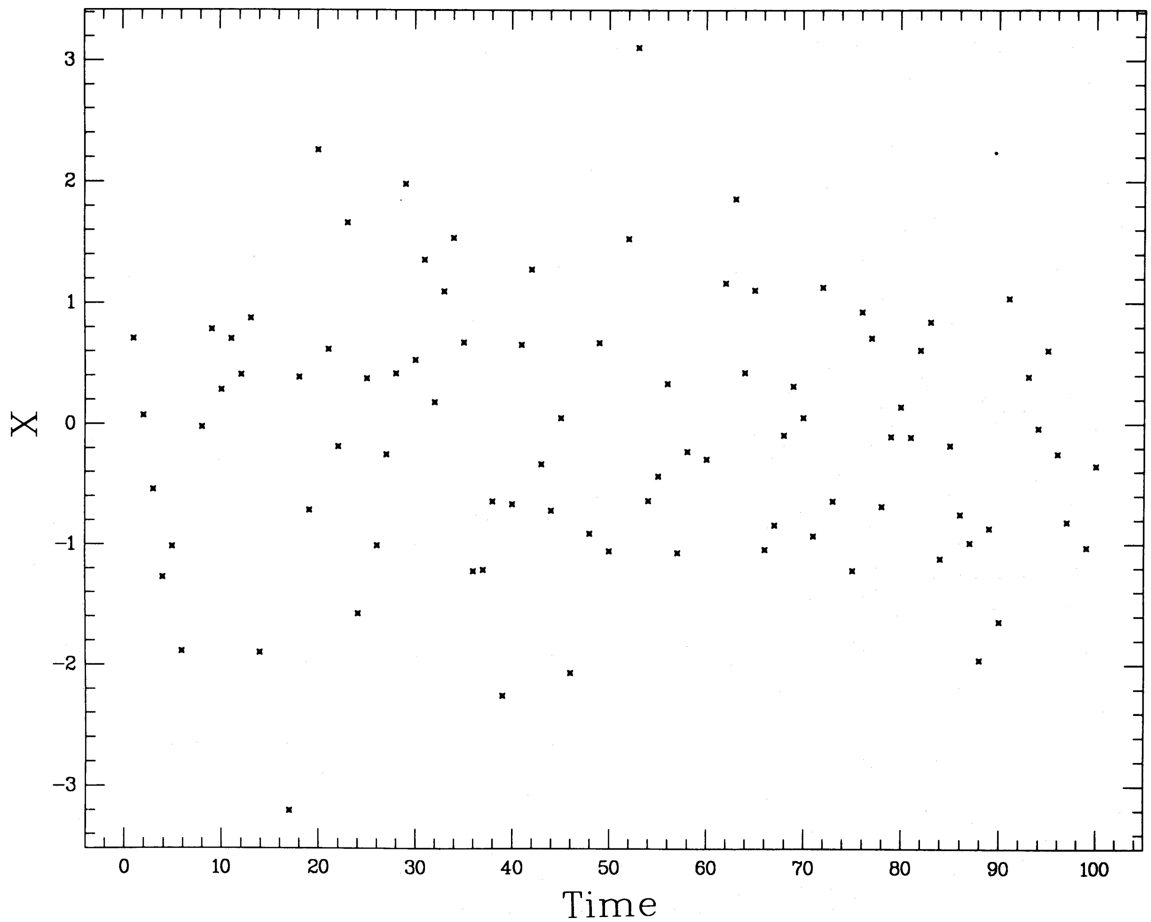

FIG. 1.—Simulated data set with $X(t) = 0.75 \cos(0.6t) + R(t)$, where $R(t)$ is Gaussian noise with variance $\sigma_r^2 = 0.902$. The period is 10.47 time units. These data have a signal-to-noise ratio of $\xi = 0.313$. The sample times are the integers between 1 and 100, with 10 integers discarded randomly. Because the signal-to-noise ratio is low, it is impossible to select the period by eye.

Also $C(\omega_{0,1}) = X_{0,1}(N_0/2)^{1/2}$ and

$$P_N(\omega_{0,1}) = \frac{N_0}{2}\left(1 + \frac{X_{1,0}^2}{X_{0,1}^2} + \frac{2\sigma_r^2}{X_{0,1}^2}\right)^{-1} . \tag{25}$$

As we add more signals, it becomes, not surprisingly, more difficult to pick out the signals. Compared to the case of a single sinusoid, the analysis of data with multiple periods will require a higher signal-to-noise ratio in order to detect peaks with the same confidence.

Some additional complications may occur when multiple frequencies are present (cf. Kovacs 1981). If the data are evenly spaced in time, then the spacing between the frequencies is $2\pi/T$ which is also conveniently at the first zero of the sine function. Each peak in the periodogram has a full width at half-maximum of $5.5662/T$. Some problems can occur if the independent frequencies are closer together than that. Any uneven spacing in the data will perturb these frequency spacings, making some closer to and some farther away from each other. If two powerful frequencies are closer than $5.5662/T$ from each other, the resultant periodogram peak will lie between them. This type of complicated peak can usually be noticed by its large width and unusual shape.

IV. SUMMARY

The modified periodogram calculated according to Scargle (1982) for unevenly sampled data is extremely valuable in assessing periodicities in astronomical time series. The likelihood of the existence of a periodic signal can be established with the false alarm probability. We have proven that the simple exponential behavior of the false alarm probability is valid *only* when the total variance of the data is used to normalize the periodogram. Other estimates of the variance, for example, the residual after a signal has been removed, will result in an incorrectly normalized exponential probability distribution. The false alarm probability can be calculated using the formula for the number of independent frequencies derived in § II*c*. This formula is accurate for evenly spaced data. The formula will overestimate the number of independent frequencies for the same data unevenly sampled. The unevenly sampled data will therefore have lower false alarm probabilities. If a data set is severely unevenly sampled, the true false alarm probability could be significantly smaller. The significance of a peak in the periodogram will be correspondingly underestimated. In this case, it can be worthwhile to determine the correct false alarm probability from a series of simulations. Properly used, the

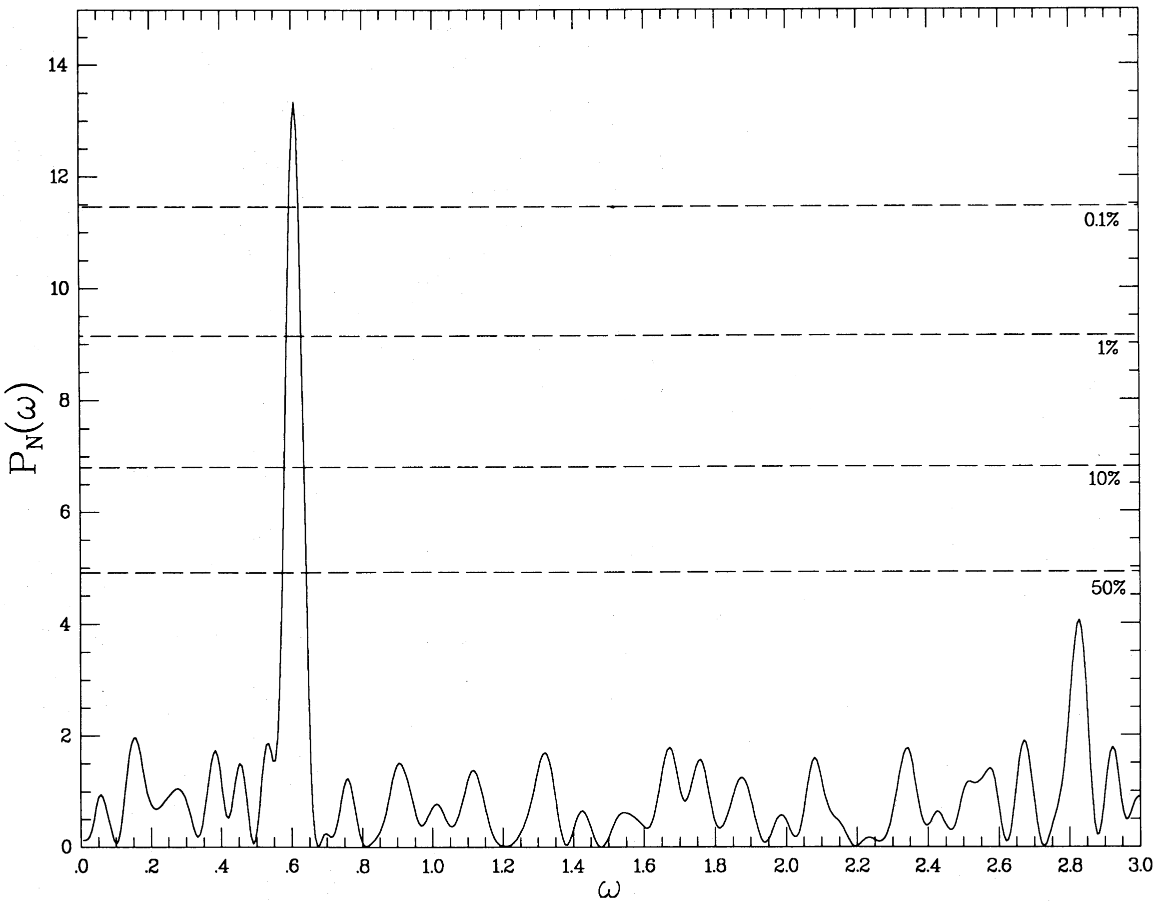

FIG. 2.—Fourier transform of the data in Fig. 1. The periodogram was calculated from $\omega = 2\pi/T$ to $\omega = \pi N_0/T$ with a spacing of about $1/T$. The highest peak is at $\omega = 0.608 \pm 0.006$ with a false probability of $F = 1.52 \times 10^{-4}$. Various false alarm probability levels are marked. Despite the low signal-to-noise ratio and the lack of a visible period in Fig. 1, the periodogram easily finds the correct period.

periodogram can detect even faint signals in noisy data. The uncertainty of a detected frequency can be evaluated easily, even when multiple signals are present.

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