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Further development and application of the spectral analysis by least squares fit

by

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1) Introduction

It was shown in Vaníček [8] that the mean-quadratic distance $\varrho(F,T^*)$ given by

$$\varrho^2 = \sum_{t\in \mathcal{M}_n} (F(t) - T^*(t))^2 , \qquad 1$$

where F is a given function defined on a set $\mathcal{M}_n$ of equidistant points, and T^* is the generalised trigonometric polynomial,

$$T^* = a_o + a \cos \omega t + b \sin \omega t \qquad 2$$

whose coefficients $\vec{a} \equiv \{a_o, a, b\}$ for any frequency ω are determined by the set of normal equations

$$M\vec{a} = \vec{l} \qquad 3$$

and $\vec{l} \equiv \{\sum_{t\in\mathcal{M}_n} F(t), \sum_{t\in\mathcal{M}_n} F(t)\cos\omega t, \sum_{t\in\mathcal{M}_n} F(t)\sin\omega t\}$, can be regarded as a transformation of F into frequency space if we take ω as free parameter. It has also been shown that such a transformation has the following useful properties :

i) If F is represented by a simple sinusoidal curve with a frequency μ then the absolute minimum of ϱ^2 is achieved for $\omega = \mu$;

ii) ϱ^2 is invariable in the transformation $F \to F +$ const.

In the present paper, we are going to show that the method can be used for analysing functions defined on any set $\mathcal{N}_n$ of unequidistant points, just as easily as a function defined on a set of equidistant points.

Further the method is adaptable to allow for cases when F is assumed to be a combination of (a) constituents of known analytical form and unknown magnitudes and (b) periodic constituents of unknown periods as well as magnitudes. The constituents of the known analytical forms will be further referred to as "known" constituents. In other words this means that the transformation can be altered in such a way that the functions, periodical or non-periodical, the presence of which is known beforehand can be used to improve the spectral image even if we do not know their magnitudes.

For simplicity, we shall be using mainly the "complement" σ of ϱ^2:

$$\sigma(\omega) = \sum_{t\in\mathcal{M}_n} F^2(t) - \varrho^2(\omega) \qquad 4$$

that gives the location of predominant frequencies in the form of maxima (peaks) instead of minima, as the former is the familiar way in the spectral analyses in general.

2) Random number tests

In order to determine whether a bias towards or against any particular frequency exists in the least squares spectrum (4), tests have been carried out using two different time series containing 599 pseudo random numbers each. These numbers have been generated from methods described in Pike and Hill [4]. The procedures for the generation of pseudo random numbers are available in the standard procedures library of the Liverpool University KDF9. The distribution of probability of the first set is normal and the second rectangular. In order to obtain comparable values in the two analyses the spectrum is plotted in the units of $\sigma/\sum F^2$ which we call proportionate variance. The results are in Fig. 1a and 1b. Few peaks are recorded in both analyses which have spectral values of magnitude surpassing 2% but within 3% of the upper limit, i.e. $\sum F^2$. Their distribution appears to have random characteristics. The appearance of these "larger" peaks may be assigned either to the short span of data or the processes by which these numbers have been generated. The larger span of data should tend to diminish the amplitudes of these peaks. Comparison of these analyses does not seem to indicate a bias towards or against any frequency.

3) Comparison with power spectrum

Power spectrum of a time series is computed from a cosine transform of auto covariances and the values thus obtained indicate the amount of energy against frequency, see for instance Blackman and Tukey [1]; whereas the least squares spectrum gives the values of the proportional variances against frequency. Thus it gives the reduction in the variance of the time series if the constituent, representing that frequency, is subtracted. The mathematical aspect of the comparison of these two methods would be complicated. Therefore it was decided to carry out comparative tests by analysing two identical time series by both the techniques. Two such tests have been realised on the different types of data. In one analysis 50 years of the monthly mean sea level of Baltimore, U.S.A., were used. In the other 256 daily values of a residual tide (observed minus predicted sea level) were analysed. For the power spectrum analysis of the mean sea level, the maximum lag of 24 months was used giving a resolution of 0·25 cycles per year. In the case of residual tide, the maximum lag used was 30 days with corresponding resolution of 0·5 cycles per month. Both power spectra were smoothed by applying "Hanning window". The computations were carried out by means of the existing Algol standard procedure of the University of Liverpool Department of Oceanography.

(a) Analysis of the Mean Sea Level of Baltimore

The power spectrum of the monthly mean sea level of Baltimore, see Fig. 2a, brings out the well known annual and semi-annual periods clearly. The lower frequencies are merged with the noise at the low frequency end of the spectrum. For fuller discussion see Rossiter [6]. The least squares spectrum, see Fig. 2d, not only locates the annual and semi-annual frequencies but at the same time it shows up a number of low frequencies. These low frequencies can be assigned to physical systems, such as 12.6 and 17.1 to being close to the periods ascribed to sunspot activity and nodal tide (see [7]). This higher power of distinction in the low frequency band has been pointed out in the references Vaníček [8], [9] already.

(b) Residual tide of Tower Pier

The data consisted of daily values of the amplitudes of the residuals. The results are in Fig. 3a and 3b. The power spectrum indicates the presence of 3, 4 and 7 day periods. The lower frequencies are once again obscured in the noise. Several long periods have been located by the least squares spectrum in addition to the periods present in the power spectrum analysis. In this analysis several of the low frequencies can be assigned to processes like seasonal changes, monthly and fortnightly tides, see Quraishee [5]. The remaining frequencies reflect most likely the interactions of different influences like numerous combinations of seasonal varying oceanic quantities such as currents, depths, ice boundaries, densities, etc.

4) Comparisons of the analyses of equi-interval and unequi-interval time series

It has been mentioned in [8] and [9] that the least square spectrum can be computed even for an unequi-interval time series. From practical aspects this possibility is very useful as in the geophysical work one often encounters the situation of discontinuous data. In order to show the influence of discontinuities on the spectral image, Baltimore monthly mean sea level data of 599 months was disjointed by deliberately removing certain data at random. Thus the total series was reduced to 559 observations. The spectrum of this series is in Fig. 2c. For comparison see the spectrum of the original continuous data in Fig. 2d. The spectral values in both cases have been normalised to give the proportionate variance. All the significant periods present in the continuous data have been brought out in the spectrum of the series of the unequi-interval data. The major peaks at yearly and half yearly periods are very well located with almost the same percentage of the total variance. Few minor peaks have shown up in the unequi-interval analysis in the flat region of the equi-interval spectrum just before half yearly period. They are insignificantly small as their magnitudes are of the order of 0·5% of the total variance. The overall impression is that both spectra are well compatible for significant periods while they vary slightly in locating insignificant ones. Experience shows that for a lesser number of values in data, side bands seem to develop around the major peaks.

5) Cases of the "known" constituents in F

Let us consider the problem when we are to estimate the unknown periods of a given real function F, defined on a set $\mathcal{N}_n$ of n scattered points and the constituents $\phi_1, \phi_2, \ldots, \phi_m$ of which are "known". These constituents may be any real functions defined for argument $t \in \mathcal{N}_n$ like $\cos \varkappa t$, $\sin \varkappa t$ (for fixed $\varkappa$), algebraic functions t^j, for $j = 1, 2, \ldots,$ exponential functions $e^{\lambda t}$ (for fixed λ), numerical functions known beforehand from earlier experiments or even functions defined separately for different parts of $\mathcal{N}_n$. The latter is the case of discontinuous datum when we can define the appropriate function as

$$\phi_i(t) = \begin{cases} 1 & \text{for } t \in \mathcal{P} \subset \mathcal{N}_n \\ 0 & \text{for } t \notin \mathcal{P}, \end{cases}$$

where $\mathcal{P}$ is the part of $\mathcal{N}_n$ in the shift of datum of which we are interested. It is not necessary to know the magnitude of the "known" constituents since these will be determined in the process of computation. If the magnitude of a constituent is known then it is better to subtract the constituent at the beginning, and disregard it from the analysis point of view completely.

Let us denote now :

$1 = \phi_{m+1}(t)$, $\cos\omega t = \phi_{m+2}(t)$, $\sin\omega t = \phi_{m+3}(t)$ and

$a_0 = a_{m+1}$, $a = a_{m+2}$, $b = a_{m+3}$

in order to achieve a uniform notation. Denoting $m+3 = N$ we can write

$$\varrho^2(\omega) = \sum_{t\in \mathcal{R}_n} \Big(F(t) - \sum_{j=1}^{N} a_j \phi_j(t)\Big)^2, \qquad 5$$

where the coefficients $\vec{a} \equiv \{a_1, a_2, \dots, a_N\}$ of the generalised polynomial $P_N = \sum_{j=1}^{N} a_j \phi_j$ are determined by the set of normal equations (3) for any ω. In this case though, M will consist of all scalar products of all the combinations of ϕ_i, ϕ_j and the right hand sides will be given by expressions :

$$\ell_i = \sum_{t\in \mathcal{R}_n} F(t)\,\phi_i(t) \;, \qquad i = 1, 2, \dots, N. \qquad 6$$

Here, of course, we assume that the system of functions $\phi \equiv \{\phi_1, \phi_2, \dots, \phi_N\}$ is, for all concerned values of ω, "linearly independent on $\mathcal{R}_n$" so that the equations (3) have unique solution for all ω. Whether this assumption is fulfilled is to be established for every individual case as it depends not only upon the choice of ϕ but on $\mathcal{R}_n$ as well.

For the complement σ we can write :

$$\sigma(\omega) = \sum_{t\in \mathcal{R}_n} \big(2F(t)P_N(t) - P_N^2(t)\big) = $$
$$= 2\sum_{j=1}^{N} a_j \sum_{t\in \mathcal{R}_n} F(t)\phi_j(t) - \sum_{t\in \mathcal{R}_n}\sum_{i=1}^{N}\sum_{j=1}^{N} a_i a_j \phi_i(t)\phi_j(t) \,. \qquad 7\cdot 1$$

Making use of (6) and substituting ℓ_i for $\sum_{j=1}^{N} a_j \sum_{t\in \mathcal{R}_n} \phi_i(t)\phi_j(t)$ from (3), we can rewrite (7.1) as follows :

$$\sigma = 2\vec{a}\vec{\ell} - \sum_{i=1}^{N} a_i \ell_i = \vec{a}\vec{\ell}. \qquad 7\cdot 2$$

Since the system ϕ is supposedly linearly independent, we can write again from (3) :

$$\sigma = (M^{-1}\vec{\ell})\,\vec{\ell} \qquad {}^{*)} \qquad 7\cdot 3$$

~~The spectrum can be computed from the above formula.~~

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*) This expression is referred to as "prediction variance" in Munk and Cartwright [3]. It shows how much the variance of F is reduced when the appropriate "prediction" is subtracted.

Denoting the minors of $\mathbf{M}$ by A_{ij} we get finally

$$\sigma = \frac{1}{\det(\mathbf{M})} \sum_{i=1}^{N} \sum_{j=1}^{N} A_{ij} \ell_i \ell_j . \qquad 7.4$$

We shall prove that providing ϕ is on $\mathcal{N}_n$ linearly independent for all concerned ω, σ is invariant in any transformation $F \rightarrow F' = F + L$ if L is a linear combination

$$L = \sum_{j=1}^{m+1} \lambda_j \phi_j \qquad 8$$

of $\phi_1, \phi_2, \ldots, \phi_{m+1}$.

Under the described circumstances, (3) gives for any F and any fixed frequency ω one best fitting polynomial $P_N = \vec{a}\vec{\phi}$. Similarly, the same system for the same frequency gives for F' a polynomial $P_N' = \vec{a}'\vec{\phi}$. Obviously, we can write for coefficients $\vec{a}'$:

$$\vec{a}' = \mathbf{M}^{-1} \vec{\ell}'. \qquad 9$$

Denoting $\sum_{t \in \mathcal{N}_n} F'(t) \phi_i(t) = \ell_i'$ we get :

$$\ell_i' = \sum_{t \in \mathcal{N}_n} F(t) \phi_i(t) + \sum_{t \in \mathcal{N}_n} L(t) \phi_i(t) = \ell_i + \Delta \ell_i , \quad i = 1, 2, \ldots, N. \qquad 10$$

Evidently, if we denote $\vec{a}' = \vec{a} + \vec{\Delta a}$ we obtain for $\vec{\Delta a}$:

$$\vec{\Delta a} = \mathbf{M}^{-1} \vec{\Delta \ell}. \qquad 11$$

Inverting (11) and substituting for $\vec{\Delta \ell}$ from (10) we can write finally :

$$\sum_{j=1}^{N} \Big(\sum_{t \in \mathcal{N}_n} \phi_i(t) \phi_j(t) \Big) \Delta a_j = \sum_{j=1}^{m+1} \Big(\sum_{t \in \mathcal{N}_n} \phi_i(t) \phi_j(t) \Big) \lambda_j , \quad i = 1, 2, \ldots, N. \qquad 12$$

Since ϕ is linearly independent we are getting :

$$\Delta a_i = \begin{cases} \lambda_i & i = 1, 2, \ldots, m+1 \\ 0 & i = m+2, m+3 \end{cases} \qquad 13$$

and therefore :

$$P_N' = P_N + L . \qquad 14$$

For the mean-quadratic distance we have :

$$\varrho(F', P_N') = \varrho(F + L, P_N + L) = \varrho(F, P_N) \qquad 15$$

and thereafter for the complements :

$$\sigma(F', P_N') = \sigma(F, P_N). \qquad 16$$

The result then shows that any transformation of F to $F + L$ as defined above does not affect the spectral image. Let us note here that from this point of view the invariability of ϱ^2 in the transformation $F \rightarrow F +$ const. is a particular case of a more general feature.

Since we are entitled to add to the analysed function F any linear combination of the "known" constituents without changing the transform σ we may as well choose such a combination that will make $l'_1, l'_2, \dots, l'_{m+1}$ equal to zero. It is not difficult to see from (10) that such a set of λ_j can be calculated from the following system of equations :

$$\sum_{j=1}^{m+1} \Big(\sum_{t\in\mathcal{N}_n} \phi_i(t)\,\phi_j(t)\Big)\lambda_j = -\sum_{t\in\mathcal{N}_n} F(t)\,\phi_i(t)\,, \qquad i = 1, 2, \dots, m+1 \qquad 17$$

which is nothing else but again the system of normal equations for coefficients of the best fitting generalised polynomial composed from the "known" functions.

Now, we can see from (7.4) that if we subtract from the given F the best fitting polynomial P_{m+1} , calculated beforehand for the "known" constituents, the transform σ' of the new function $F' = F - P_{m+1}$ will be identical with the initial σ although the formula for numerical computation will become far simpler :

$$\sigma' = \sigma^{*} = \frac{1}{\det(\mathbf{M})} \sum_{i=m+2}^{N} \sum_{j=m+2}^{N} A_{ij}\, l'_i\, l'_j \qquad 18.1$$

Considering the described reduction of F as part of the whole process we can finally write for σ the following expression :

$$\sigma(\omega) = p(\omega)\Big(\sum_{t\in\mathcal{N}_n} F'(t)\cos\omega t\Big)^2 + q(\omega)\Big(\sum_{t\in\mathcal{N}_n} F'(t)\sin\omega t\Big)^2 + r(\omega)\sum_{t\in\mathcal{N}_n} F'(t)\cos\omega t \sum_{t\in\mathcal{N}_n} F'(t)\sin\omega t \qquad 18.2$$

where p, q, r are real, non-negative functions of ω depending on the "known" constituents and $\mathcal{N}_n$.

Formula (18.2) is valid for any $\mathcal{N}_n$ since we have not limited ourselves to any particular case and can thus be used for analysing any time series $\{F(t);\, t\}$ either equidistant or unequidistant. For equiddistant time series though, the functions p, q, r acquire simpler form because the summation over t in individual scalar products can usually be expressed by simpler formulae. In addition to this, if the "known" as well as sought functions, i.e. $\phi_1, \phi_2, \dots, \phi_{m+1}, \phi_{m+2}, \phi_N$, are either even or odd on $\mathcal{N}_n$, $r(\omega)$ becomes zero. .

6) <u>Treatment of functions containing trend</u>

The simplest and most obvious application of the possibilities described in § 5 is the treatment for functions containing trend, which is a very common case in all geophysical sciences. We shall regard trend as linear term of unknown magnitude and for simplicity, consider $\mathcal{N}_n \equiv \mathcal{M}_n \equiv \{-\pi + \frac{2\pi}{n-1}(i-1)\}$,

$i=1,2,\dots,n$, n odd. Beside this, let us agree that symbol Σ will mean summation over $t\in\mathcal{M}_n$ if not stated otherwise.

In accordance with § 5, we shall begin with subtracting the term C_1+C_2t from the original function F. The coefficients C_1, C_2 can be determined from the following system of equations (see 17) :

$$\begin{aligned} nC_1 + \Sigma t\cdot C_2 &= \Sigma F(t) \\ \Sigma t\cdot C_1 + \Sigma t^2\cdot C_2 &= \Sigma tF(t). \end{aligned} \qquad 19$$

Since the functions 1 and t are on $\mathcal{M}_n$ obviously linearly independent, we get one solution only, which can be written, due to our choice of $\mathcal{M}_n$ Σt becomes 0, as follows :

$$C_1 = \frac{1}{n}\Sigma F(t) = \bar{F} \qquad 20.1$$

$$C_2 = \Sigma tF(t)/\Sigma t^2. \qquad 20.2$$

For computation purpose, the latter equation can be rewritten, considering the relations :

$$\Sigma t^2 = \frac{n\pi^2}{3}\frac{n+1}{n-1}, \quad \Sigma tF(t) = -\pi\frac{n+1}{n-1}\Sigma F(t) + \frac{2\pi}{n-1}\sum_{i=1}^{n} iF(t_i) \qquad 21$$

as follows :

$$C_2 = -\frac{3}{\pi}C_1 + \frac{6}{\pi n(n+1)}\sum_{i=1}^{n} iF(t_i). \qquad 20.3$$

Due to the choice of $\mathcal{M}_n$ again, functions $\phi_1(t)=t$, $\phi_4(t)=\sin\omega t$ are on $\mathcal{M}_n$ even and $\phi_2(t)=1$, $\phi_3(t)=\cos\omega t$ are odd. Thus the matrix $\mathbf{M}$ of the system of normal equations degenerates into two independent matrices $\mathbf{M}_E$ and $\mathbf{M}_\sigma$ containing the scalar products of odd and even functions only respectively :

$$\mathbf{M} = \left\|\begin{matrix} \Sigma\phi_1\phi_1 & 0 & 0 & \Sigma\phi_1\phi_4 \\ 0 & \Sigma\phi_2\phi_2 & \Sigma\phi_2\phi_3 & 0 \\ 0 & \Sigma\phi_3\phi_2 & \Sigma\phi_3\phi_3 & 0 \\ \Sigma\phi_1\phi_4 & 0 & 0 & \Sigma\phi_4\phi_4 \end{matrix}\right\| = \left\|\begin{matrix} \mathbf{M}_E, & 0 \\ 0, & \mathbf{M}_\sigma \end{matrix}\right\|. \qquad 22$$

Thus we get for the relevant minors :

$$\begin{aligned} A_{33} &= \Sigma\phi_2\phi_2 \det(\mathbf{M}_E) = n \det(\mathbf{M}_E) \\ A_{34} &= 0 \\ A_{44} &= \Sigma\phi_1\phi_1 \det(\mathbf{M}_\sigma) = \Sigma t^2 \det(\mathbf{M}_\sigma). \end{aligned} \qquad 23$$

According to Laplace theorem (see for instance Fadejev, Fadejeva [2]), we can write for $\mathbf{M}$:

$$\det(\mathbf{M}) = \det(\mathbf{M}_\sigma)\cdot\det(\mathbf{M}_E)$$

so that the formula 18.1, after substituting for $\det(\mathbf{M}_\sigma)$ and $\det(\mathbf{M}_E)$, will be as follows :

$$\sigma = \frac{(\Sigma F(t)\cos\omega t)^2}{\Sigma\cos^2\omega t - \frac{1}{n}(\Sigma\cos\omega t)^2} + \frac{(\Sigma F(t)\sin\omega t)^2}{\Sigma\sin^2\omega t - \frac{3(n-1)}{\pi^2 n(n+1)}(\Sigma t\sin\omega t)^2}. \qquad 25$$

In this final formula the denominators are functions of ω only (as stated in § 5) and can be obviously expressed in more convenient form for computation. It can be proved that both denominators are positive for $\omega \in (0, \frac{1}{4}(n-1))$.

7) Comparison of analyses with and without excluding trend

Two different geophysical time series were selected for showing the effect of introducing one "known" constituent in the analysis, in this case the secular trend. They are 60 years of monthly mean sea level observations of Baltimore and 159 days of hourly tilt observations realised by means of O.R.B. 88 quartz horizontal pendulum set up in N/S direction in the basement of Bidston Observatory (Cheshire, England).

(a) The Mean Sea Level of Baltimore

The spectrum of Baltimore mean sea level with the trend excluded is in Fig. 2b. The effect of the consideration, comparing with Fig. 2d, is most obvious for the low frequency peaks. The lowest frequency in d) is suppressed and shifted towards the high frequency side. The other low frequencies are also shifted slightly (17.1 → 16.9 years, 12.6 → 13.2, 10.0 → 9.9, 6.8 → 7.2) while the image as a whole is more pronounced, especially for strong periods. Note the annual period in particular.

(b) The Earth Crust Tilt

Three frequency bands - low, diurnal, semidiurnal - of the spectrum are shown in Fig. 4a, 4b, 4c. To convey clearer meaning the spectrum this time is plotted in units of "normalised variance", i.e. σ/n. Spectrum with trend included is plotted in dotted line, with trend excluded in plain. The effect of excluding trend is marked again in the intensification of major peaks; note particularly the split in peak corresponding to the combination of S_1, P_1, K_1 waves. The low frequency band is noticable for the presence of weekly period, fortnightly tide and several periods in the vicinity of one month - see Vaníček [9] [10]. The largest peak which is not fully shown in Fig. 4a may be attributed to the large yearly constituent usually present in tilt observations - see again Vaníček [9] [10].

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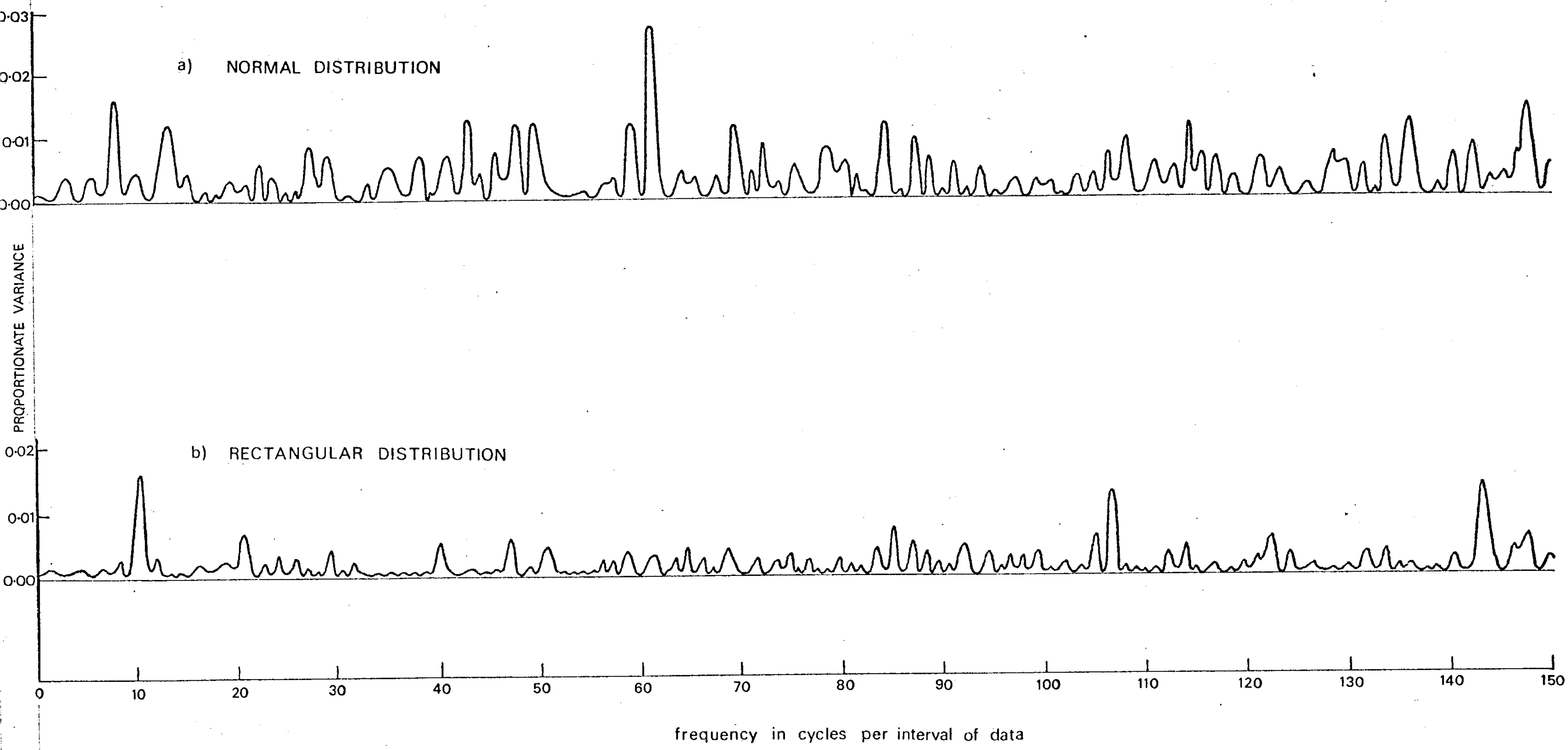
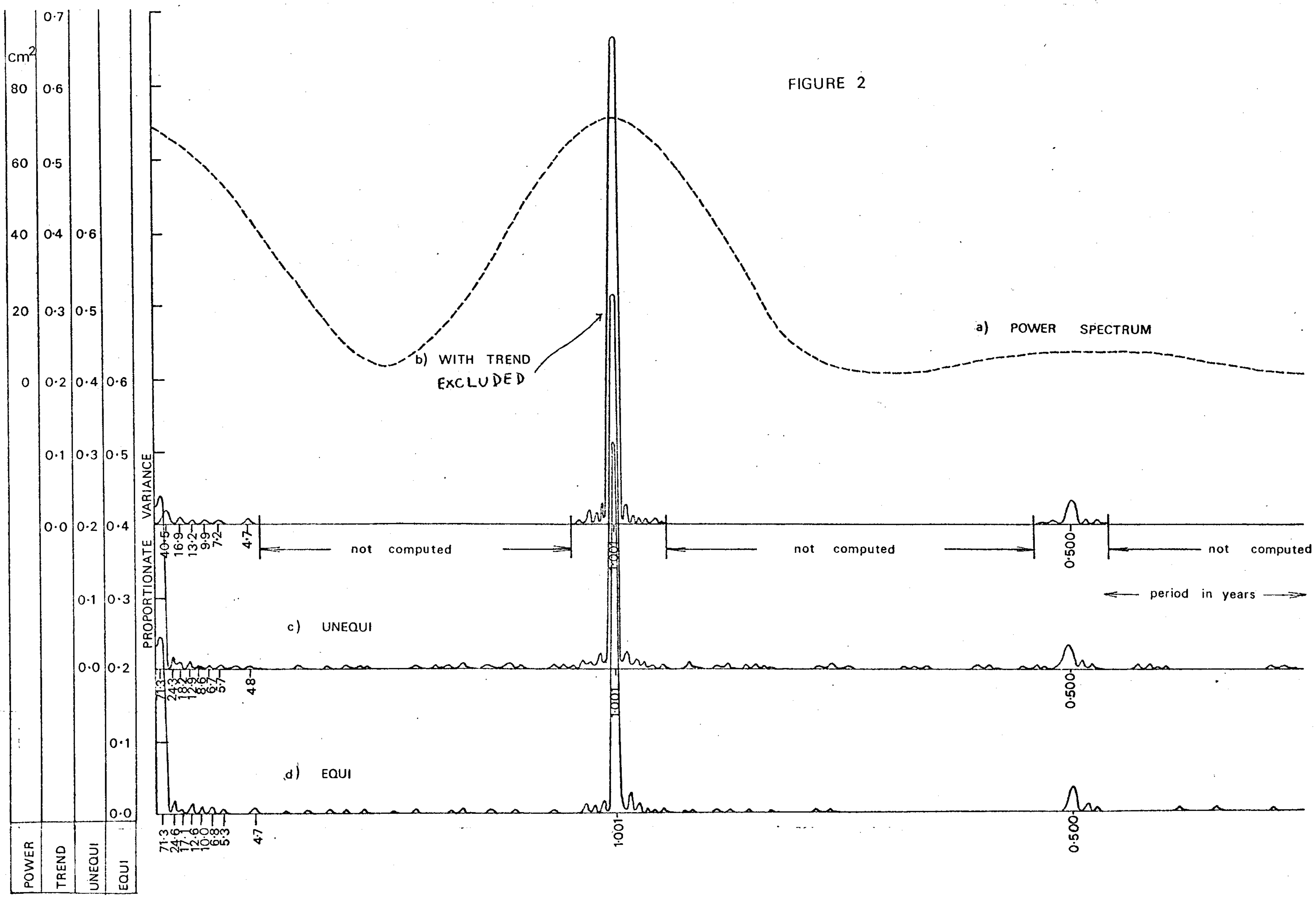
FIGURE 1



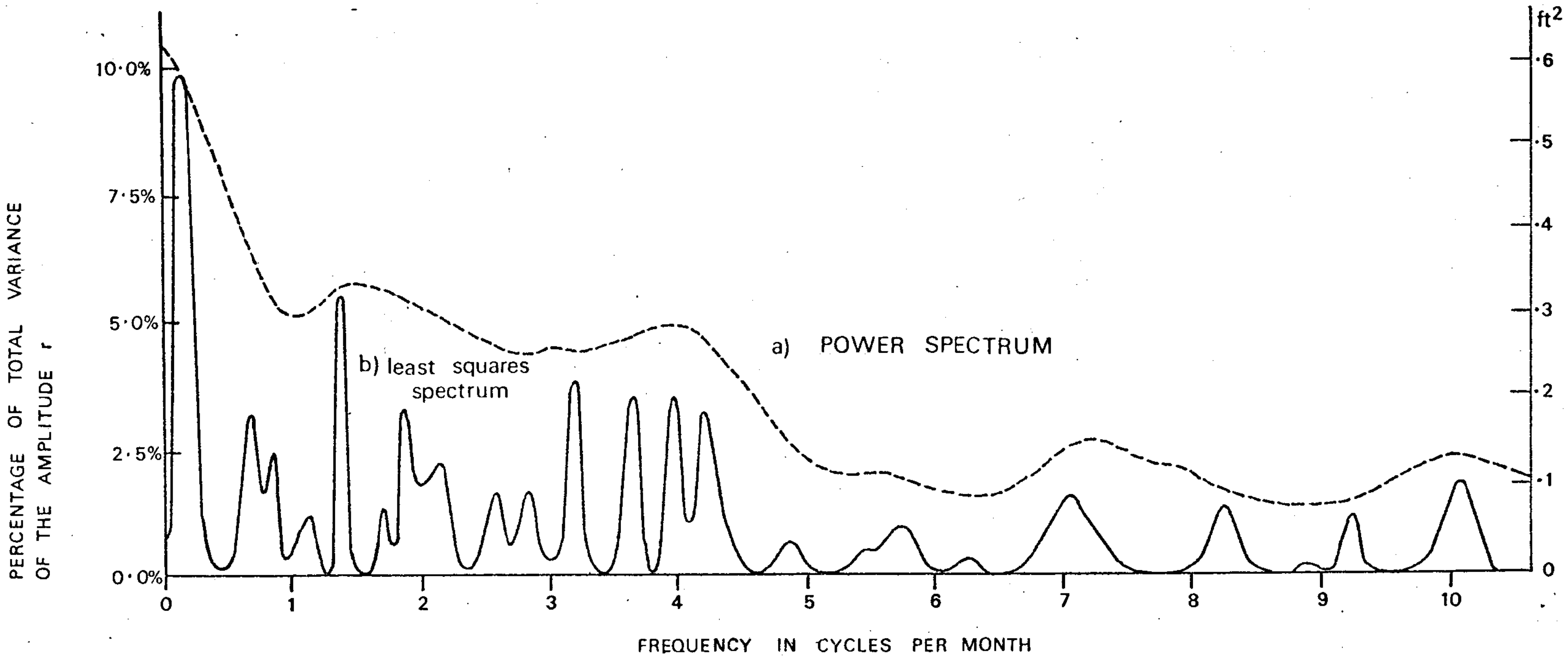
a) NORMAL DISTRIBUTION
b) RECTANGULAR DISTRIBUTION
PROPORTIONATE VARIANCE
0·03
0·02
0·01
0·00
0·02
0·01
0·00
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
frequency in cycles per interval of data

FIGURE 2



a) POWER SPECTRUM
b) WITH TREND EXCLUDED
c) UNEQUI
d) EQUI
PROPORTIONATE VARIANCE
POWER
TREND
UNEQUI
EQUI
cm2
not computed
period in years

FIGURE 3


PERCENTAGE OF TOTAL VARIANCE
OF THE AMPLITUDE r
10·0%
7·5%
5·0%
2·5%
0·0%
b) least squares
spectrum
a) POWER SPECTRUM
ft²
·6
·5
·4
·3
·2
·1
0
0
1
2
3
4
5
6
7
8
9
10
FREQUENCY IN CYCLES PER MONTH

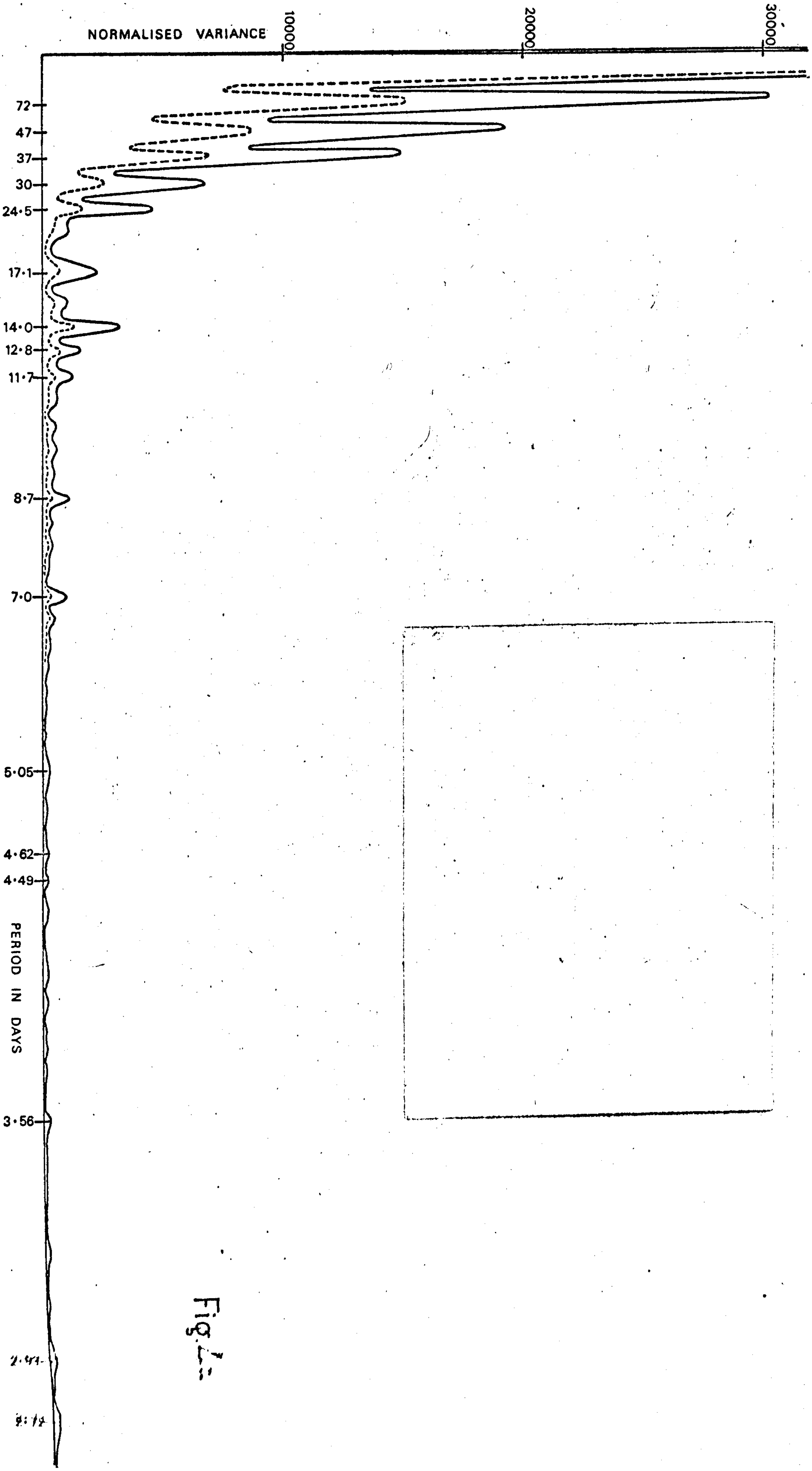

NORMALISED VARIANCE
10000
20000
30000
72
47
37
30
24·5
17·1
14·0
12·8
11·7
8·7
7·0
5·05
4·62
4·49
3·56
PERIOD IN DAYS

Fig. 2

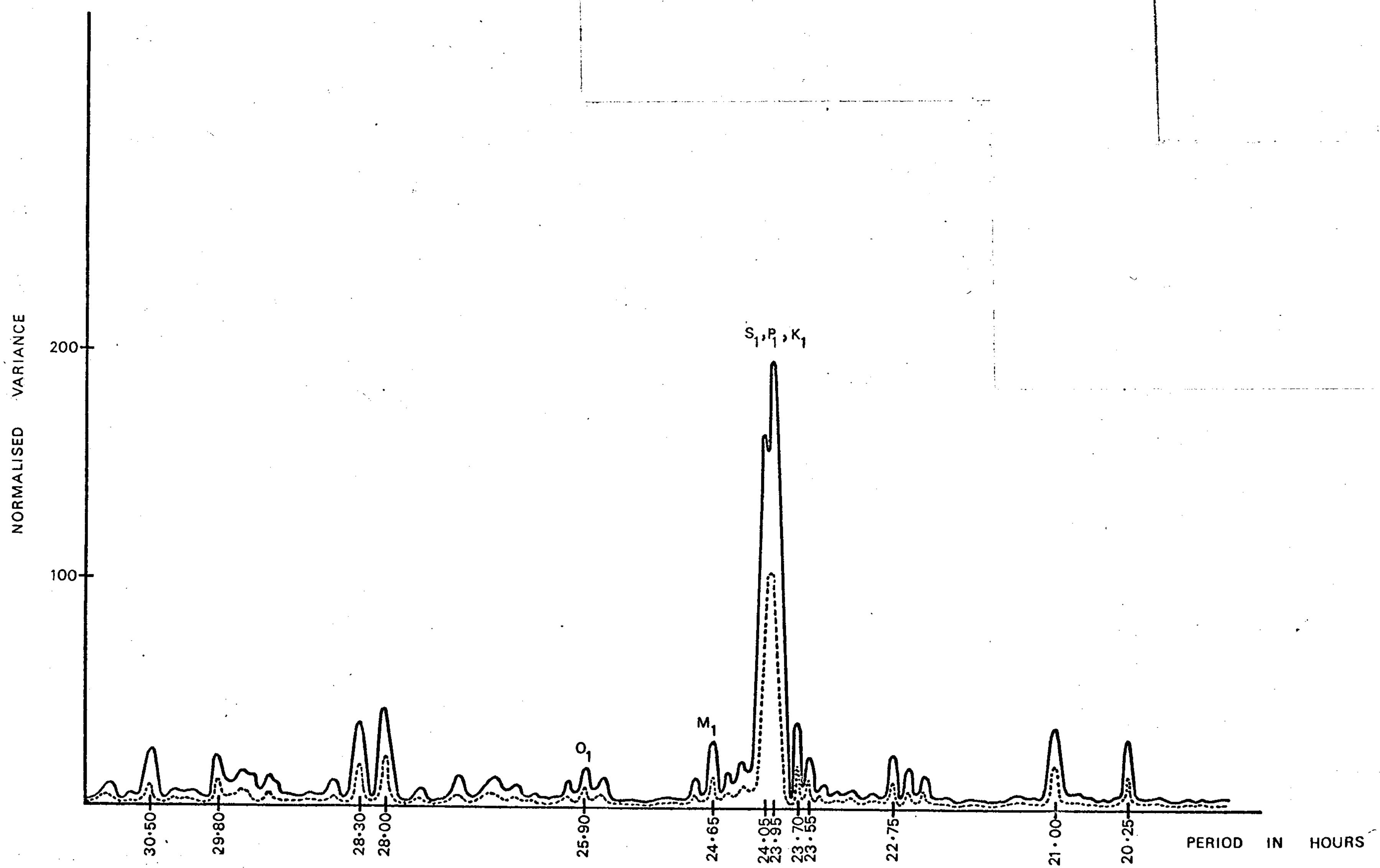

NORMALISED VARIANCE
100
200
S_1, P_1, K_1
M_1
O_1
30·50
29·80
28·30
28·00
25·90
24·65
24·05
23·95
23·70
23·55
22·75
21·00
20·25
PERIOD IN HOURS

Fig. 4b

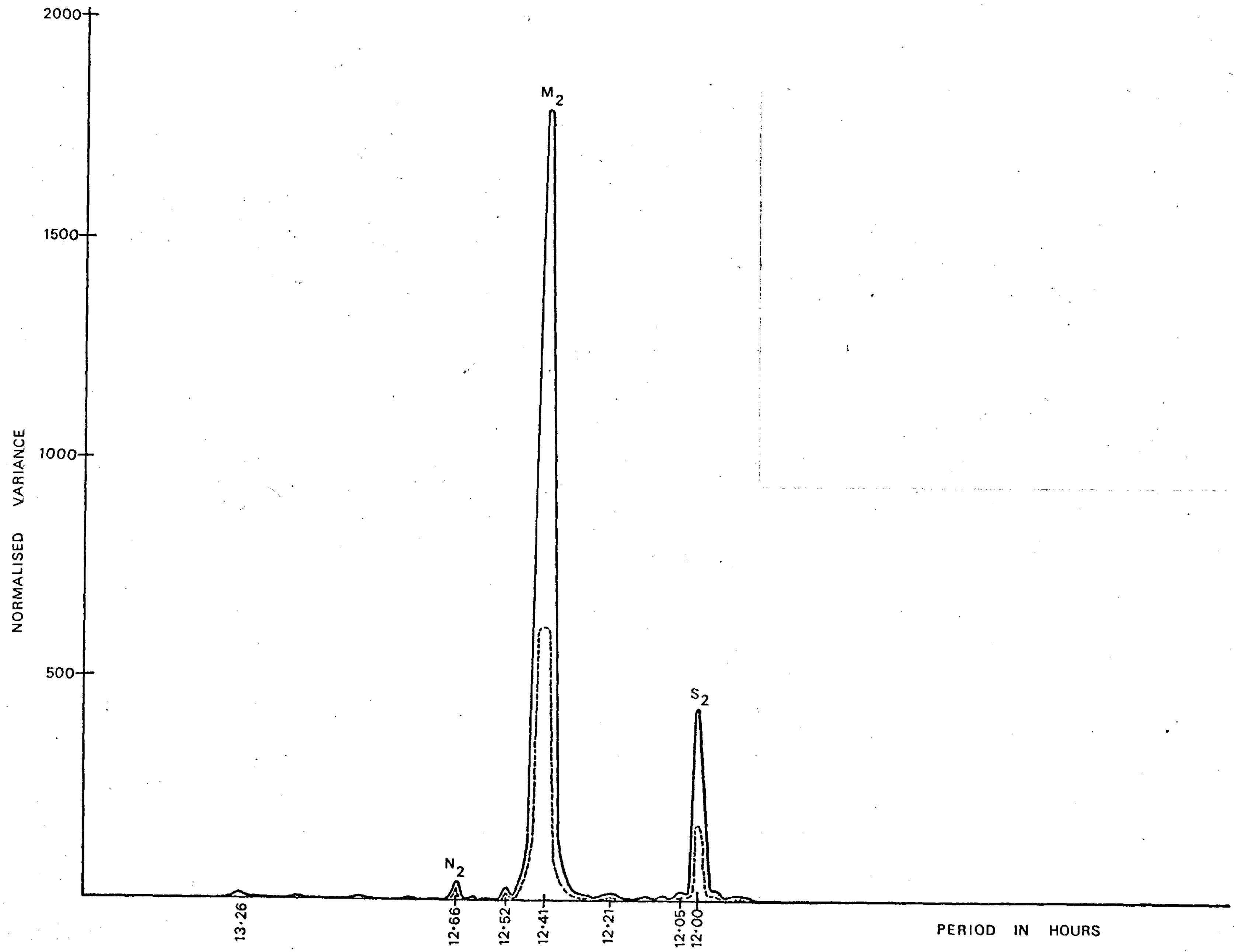

NORMALISED VARIANCE
2000
1500
1000
500
M_2
N_2
S_2
13·26
12·66
12·52
12·41
12·21
12·05
12·00
PERIOD IN HOURS

Fig. 4c