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SCHOOL ON PHYSICAL METHODS FOR THE STUDY OF THE UPPER AND LOWER ATMOSPHERE SYSTEM

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The Search for Periodicity

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2

THE SEARCH FOR PERIODICITY

In this chapter we examine the problem of describing what periodicities if any are present in a given set of data. In some cases we know a collection of periods that may be expected to be present, and we have to find the associated amplitudes and phases. However, often we have no prior information about the periods, and these too must be found. The first problem is simpler, and we discuss it first. From this discussion we shall develop a way of solving the more difficult problem.

2.1 A CURVE-FITTING APPROACH

As an example consider the variable-star data of Figure 1.1. Over the 600 days of data we count 21 peaks; this suggests that any periodicity should have a period of around $600/21 \approx 28.6$ days. Thus the t th data value should contain a component of the form $R \cos(\omega t + \phi)$, where $\omega = 2\pi/28.6 \approx 0.220$. We model the data as

$$x_t = \mu + R \cos(\omega t + \phi) + \epsilon_t, \quad t = 0, 1, \dots, 599, \quad (1)$$

the simplest case of the "hidden periodicities" model. Here x_t denotes the t th data value, and ϵ_t is the t th *residual* (that is, whatever is needed to make the equality exact). We regard the model as good (and say that it *fits* the

data well) if the residuals are generally small. The term μ is an added constant. Since a cosine wave oscillates about 0, while the data oscillate between 0 and around 30, such a term is clearly needed if the residuals are to be at all small.

The unknown parameters are μ , R , and ϕ , and in the next section we show how to find values for them that make the residuals as small as possible in a certain specific sense. Initially we shall keep ω fixed at 0.220, but in Section 2.3 we shall regard it as an additional unknown and find a better value.

For the purposes of this chapter, we shall follow the common practice of measuring the size of the residuals by the sum of their squared values. Thus the problem is to find μ , R , and ϕ (and, later ω) to minimize

$$S(\mu, R, \phi) = S(\mu, R, \phi, \omega) = \sum_{i=0}^{599} \{x_i - \mu - R \cos(\omega t + \phi)\}^2,$$

the term between braces being precisely the i th residual for given values of μ , R , and ϕ (and ω). This is an example of the method of *least squares*. Least squares methods are widely used and have many computational and theoretical advantages. However, they also have certain deficiencies, which will be mentioned briefly in Section 5.3.

It is easily seen that least squares problems are simplest when the model is a linear function of the unknown parameters, since then the function to be minimized is quadratic. Equation 1 is nonlinear in R and ϕ , but may be rewritten as

$$x_i = \mu + A \cos \omega t + B \sin \omega t + \varepsilon_i,$$

where $A = R \cos \phi$ and $B = -R \sin \phi$. Furthermore, given any values of A and B , we may solve for R and ϕ . We may therefore regard A and B as the parameters, and the model is now linear, for fixed ω . In the next section we solve the elementary problem of finding μ , A , and B for fixed ω . In Section 2.3 we show how our current estimate of the frequency ω may be improved.

Exercise 2.1 Least Squares Straight Line

Suppose that $(x_1, y_1), \dots, (x_n, y_n)$ are a set of points in the plane. It is sometimes useful to model such a set of points by a straight line, $y = a + bx$. The *least squares straight line* has parameters \hat{a} and \hat{b} which minimize

2.2 Least Squares Estimation of Amplitude and Phase

the sum of squared residuals,

$$S(a, b) = \sum_{i=1}^n (y_i - a - bx_i)^2.$$

(i) Verify that, provided the x -values are not all the same,

$$\hat{b} = \frac{\sum_{i=1}^n y_i(x_i - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

and

$$\hat{a} = \bar{y} - \hat{b}\bar{x},$$

where $\bar{x} = (x_1 + x_2 + \dots + x_n)/n$, and \bar{y} is similarly defined.

(ii) Find the corresponding formulas for the coefficients of the least squares parabola, $y = a + bx + cx^2$.

2.2 LEAST SQUARES ESTIMATION OF AMPLITUDE AND PHASE

In this section we show how to estimate the parameters of a sinusoid, with or without an added constant. The frequency ω is regarded as known and is not varied to improve the fit. In the next section the method is extended to include the estimation of ω . We consider first the simple two-parameter model of a sinusoid with no added constant. The model is

$$x_i = A \cos \omega t + B \sin \omega t + \varepsilon_i,$$

and the principle of least squares leads us to minimize

$$T(A, B) = \sum_{i=0}^{n-1} (x_i - A \cos \omega t - B \sin \omega t)^2,$$

restricting μ to be zero for the present, and keeping ω fixed. Now

$$\frac{\partial T}{\partial A} = -2 \sum \cos \omega t (x_i - A \cos \omega t - B \sin \omega t),$$

$$\frac{\partial T}{\partial B} = -2 \sum \sin \omega t (x_i - A \cos \omega t - B \sin \omega t),$$

and the equations that result from equating these to zero have the solution

$$\begin{aligned} A = \hat{A} &= \frac{1}{\Delta} \left\{ \sum x_i \cos \omega t \sum (\sin \omega t)^2 \right. \\ &\quad \left. - \sum x_i \sin \omega t \sum \cos \omega t \sin \omega t \right\}, \\ B = \hat{B} &= \frac{1}{\Delta} \left\{ \sum x_i \sin \omega t \sum (\cos \omega t)^2 \right. \\ &\quad \left. - \sum x_i \cos \omega t \sum \cos \omega t \sin \omega t \right\}, \end{aligned} \quad (2)$$

where

$$\Delta = \sum (\cos \omega t)^2 \sum (\sin \omega t)^2 - \left(\sum \cos \omega t \sin \omega t \right)^2.$$

The sums involving only trigonometric functions may be evaluated, using the results of Exercise 2.2, to give

$$\begin{aligned} \sum (\cos \omega t)^2 &= \frac{n}{2} \{ 1 + D_n(2\omega) \cos(n-1)\omega \}, \\ \sum \cos \omega t \sin \omega t &= \frac{n}{2} D_n(2\omega) \sin(n-1)\omega, \\ \sum (\sin \omega t)^2 &= \frac{n}{2} \{ 1 - D_n(2\omega) \cos(n-1)\omega \}, \end{aligned}$$

where

$$D_n(\omega) = \frac{\sin n\omega/2}{n \sin \omega/2}$$

is a version of the *Dirichlet kernel* (Titchmarsh, 1939, p. 402). The sums involving $\{x_i\}$ usually have to be evaluated directly.

To find R and ϕ , the amplitude and phase, we solve the equations $A = R \cos \phi$ and $B = -R \sin \phi$. Since R is nonnegative, it follows that $R = (A^2 + B^2)^{1/2}$. The basic equation for ϕ is $\tan \phi = -B/A$. However, the solution $\phi = \arctan -B/A$ is incorrect, since this gives the same value for $-A$ and $-B$ as for A and B . The full solution is as follows:

$$\phi = \begin{cases} \arctan(-B/A), & A > 0, \\ \arctan(-B/A) - \pi, & A < 0, B > 0, \\ \arctan(-B/A) + \pi, & A < 0, B < 0, \\ -\pi/2, & A = 0, B > 0, \\ \pi/2, & A = 0, B < 0, \\ \text{arbitrary}, & A = 0, B = 0. \end{cases}$$

(The FORTRAN function ATAN2($-B, A$) returns the required value.)

The model that seems appropriate for the variable-star data is the three-parameter "sinusoid plus constant" model given in Section 2.1,

$$x_i = \mu + A \cos \omega t + B \sin \omega t + \varepsilon_i.$$

The equations for the least squares estimates of μ , A , and B (which we shall denote as $\hat{\mu}$, \hat{A} , and \hat{B} , respectively) are

$$\begin{aligned} \sum (x_i - \mu - A \cos \omega t - B \sin \omega t) &= 0, \\ \sum \cos \omega t (x_i - \mu - A \cos \omega t - B \sin \omega t) &= 0, \\ \sum \sin \omega t (x_i - \mu - A \cos \omega t - B \sin \omega t) &= 0. \end{aligned} \quad (3)$$

These too may be solved explicitly (see Exercise 2.3). For the variable-star data with $\omega = 0.220$, we find

$$\hat{\mu} = 17.11, \quad \hat{A} = -1.102, \quad \hat{B} = 8.406,$$

and hence the estimates of R and ϕ are

$$\hat{R} = 8.478, \quad \hat{\phi} = -1.701.$$

Note that for negative $\hat{\phi}$ the argument $\omega t + \hat{\phi}$ of $\cos(\omega t + \hat{\phi})$ first vanishes at $t = |\hat{\phi}|/\omega \approx 7.7$. Thus the fitted cosine wave has a peak at $t = 7.7$, while the first peak in the data is between $t = 4$ and $t = 5$. Since the peaks in the data are not evenly spaced, this seems to be reasonable agreement.

We can find very useful approximations to (3) as follows (see Exercise 2.4). When the purely trigonometric sums are evaluated, the coefficients in (3) involve the term $n/2$ and terms such as $(n/2)D_n(\omega/2)$. We note first that $D_n(2k\pi/n) = 0$ for any integer k , and that $|nD_n(\omega)| \leq 1/(\sin \omega/2)$. This means that the terms in (3) involving D_n are, for large n and ω not too close to 0, always small compared with $n/2$, and sometimes exactly 0. By omitting all these terms we find the reduced set of equations

$$\begin{aligned} n\mu &= \sum x_i, \\ \frac{nA}{2} &= \sum x_i \cos \omega t, \\ \frac{nB}{2} &= \sum x_i \sin \omega t. \end{aligned}$$

(We note in passing that the second and third equations are also approximations to the two-parameter equations (2).)

It often happens that μ is larger than A or B , and in this case it is unwise to ignore any term involving μ . The approximations are then

$$\begin{aligned} n\mu &= \sum x_i, \\ \mu \sum \cos \omega t + \frac{nA}{2} &= \sum x_i \cos \omega t, \\ \mu \sum \sin \omega t + \frac{nB}{2} &= \sum x_i \sin \omega t. \end{aligned} \quad (4)$$

The solutions to these equations (denoted as $\tilde{\mu}, \tilde{A}, \tilde{B}$) are

$$\begin{aligned} \tilde{\mu} &= \bar{x} = \frac{1}{n} \sum x_i, \\ \tilde{A} &= \frac{2}{n} \sum (x_i - \bar{x}) \cos \omega t, \\ \tilde{B} &= \frac{2}{n} \sum (x_i - \bar{x}) \sin \omega t, \end{aligned} \quad (5)$$

and may be regarded as approximate solutions to (3) (see Exercise 2.4). For the variable-star data we find $\tilde{\mu} = \bar{x} = 17.11$, $\tilde{A} = 1.103$, $\tilde{B} = 8.403$, $\tilde{R} = 8.475$, and $\tilde{\phi} = -1.701$. Notice that the differences between these values and the exact least squares values appear only in the fourth significant figure, if at all.

The adequacy of the model as a representation of the data may be assessed by examining the sum of squares of the residuals. The values of $T(\tilde{\mu}, \tilde{A}, \tilde{B})$ and $T(\bar{x}, \tilde{A}, \tilde{B})$ are both 26,769.5, to six significant figures. The approximate solutions are very satisfactory, in that the sum of squares is increased by less than one part in a million. Either value may be compared with $T(\bar{x}, 0, 0) = 48,324.3$, the sum of squares of the residuals just from a constant term. The difference $T(\bar{x}, 0, 0) - T(\tilde{\mu}, \tilde{A}, \tilde{B}) = 21,554.8$ [or $T(\bar{x}, 0, 0) - T(\bar{x}, \tilde{A}, \tilde{B})$] may be regarded as the amount of squared variation in the data that can be accounted for by the frequency ω . A set of approximations similar to those used to obtain (5) shows that both quantities are approximately

$$\frac{n}{2} (\tilde{A}^2 + \tilde{B}^2) = \frac{n}{2} \tilde{R}^2 = 21,546.8.$$

(See Exercise 2.5.) The error in using this approximation is therefore around 3 parts in 10,000, in the present case.

Exercise 2.2 Some Trigonometric Identities

(i) Show that

$$\begin{aligned} \sum_{i=0}^{n-1} \exp(i\lambda t) &= \frac{\exp(in\lambda) - 1}{\exp(i\lambda) - 1} \\ &= \exp\left\{\frac{i(n-1)\lambda}{2}\right\} \frac{\exp(in\lambda/2) - \exp(-in\lambda/2)}{\exp(i\lambda/2) - \exp(-i\lambda/2)}. \end{aligned}$$

(ii) Use the Euler relation

$$\exp(i\lambda) = \cos \lambda + i \sin \lambda$$

and its inverse

$$\cos \lambda = \frac{1}{2} \{ \exp(i\lambda) + \exp(-i\lambda) \}, \quad \sin \lambda = \frac{1}{2i} \{ \exp(i\lambda) - \exp(-i\lambda) \}$$

to deduce that

$$\begin{aligned} \sum \cos \lambda t &= \cos \left\{ \frac{(n-1)\lambda}{2} \right\} \frac{\sin n\lambda/2}{\sin \lambda/2}, \\ \sum \sin \lambda t &= \sin \left\{ \frac{(n-1)\lambda}{2} \right\} \frac{\sin n\lambda/2}{\sin \lambda/2}. \end{aligned}$$

(iii) Use the addition formulas

$$\sin(\lambda + \mu) = \sin \lambda \cos \mu + \cos \lambda \sin \mu,$$

$$\cos(\lambda + \mu) = \cos \lambda \cos \mu - \sin \lambda \sin \mu,$$

and their inverses

$$\cos \lambda \cos \mu = \frac{1}{2} \{ \cos(\lambda + \mu) + \cos(\lambda - \mu) \},$$

$$\cos \lambda \sin \mu = \frac{1}{2} \{ \sin(\lambda + \mu) - \sin(\lambda - \mu) \},$$

$$\sin \lambda \sin \mu = \frac{1}{2} \{ \cos(\lambda - \mu) - \cos(\lambda + \mu) \},$$

to evaluate $\sum \cos \lambda t \cos \mu t$, $\sum \cos \lambda t \sin \mu t$, and $\sum \sin \lambda t \sin \mu t$. Note the special cases $\lambda = \mu$.

Exercise 2.3 Equations for the Three-Parameter "Sinusoid Plus Constant" Model

The derivatives of

$$T(\mu, A, B) = \sum_{i=0}^{n-1} (x_i - \mu - A \cos \omega t - B \sin \omega t)^2$$

with respect to μ , A , and B are

$$\frac{\partial T}{\partial \mu} = -2 \sum (x_i - \mu - A \cos \omega t - B \sin \omega t),$$

$$\frac{\partial T}{\partial A} = -2 \sum \cos \omega t (x_i - \mu - A \cos \omega t - B \sin \omega t),$$

$$\frac{\partial T}{\partial B} = -2 \sum \sin \omega t (x_i - \mu - A \cos \omega t - B \sin \omega t),$$

respectively. Simplify these expressions using the results of Exercise 2.2, and solve them for the least squares estimates $\hat{\mu}$, \hat{A} , and \hat{B} of μ , A , and B , respectively.

Exercise 2.4 The Approximate Least Squares Estimates

(i) For the two-parameter model (equations 2), show that

$$\left| \hat{A} - \frac{2}{n} \sum x_i \cos \omega t \right| = |D_n(2\omega)| |\hat{A} \cos(n-1)\omega + \hat{B} \sin(n-1)\omega|$$

$$< \frac{\hat{R}}{n \sin \omega},$$

and that similarly

$$\left| \hat{B} - \frac{2}{n} \sum x_i \sin \omega t \right| < \frac{\hat{R}}{n \sin \omega}.$$

(ii) For the three-parameter model (equations 3), show that

$$|\hat{\mu} - \bar{x}| < \frac{\hat{R}}{n \sin \omega/2}$$

and that both

$$\left| \hat{A} - \frac{2}{n} \sum x_i \cos \omega t \right| \quad \text{and} \quad \left| \hat{B} - \frac{2}{n} \sum x_i \sin \omega t \right|$$

2.2 Least Squares Estimation of Amplitude and Phase

are bounded by

$$\frac{2\hat{\mu}}{n \sin \omega/2} + \frac{\hat{R}}{n \sin \omega}.$$

(iii) For the three-parameter model show that both $|\hat{A} - \tilde{A}|$ and $|\hat{B} - \tilde{B}|$ are bounded by

$$\hat{R} \left\{ \frac{2}{(n \sin \omega/2)^2} + \frac{1}{n \sin \omega} \right\}.$$

Exercise 2.5 The Sum of Squares Associated with ω

(i) For the two-parameter model, show that

$$T(0, \hat{A}, \hat{B}) = \sum x_i^2 - \left\{ \left(\sum y_i \cos \omega t \right)^2 \sum (\sin \omega t)^2 \right.$$

$$- 2 \sum y_i \cos \omega t \sum y_i \sin \omega t \sum \cos \omega t \sin \omega t$$

$$\left. + \left(\sum y_i \sin \omega t \right)^2 \sum (\cos \omega t)^2 \right\} / \Delta.$$

NOTE: This may be interpreted as

sum of squares of residuals

= sum of squares of original data

– sum of squares associated with frequency ω .

(ii) Find the corresponding expression for the residual sum of squares $T(\hat{\mu}, \hat{A}, \hat{B})$ in the three-parameter model.

(iii) Show that the sum of squares associated with ω is approximately

$$\frac{2}{n} \left\{ \left(\sum x_i \cos \omega t \right)^2 + \left(\sum x_i \sin \omega t \right)^2 \right\}$$

in the two-parameter model, and

$$\frac{2}{n} \left[\left\{ \sum (x_i - \bar{x}) \cos \omega t \right\}^2 + \left\{ \sum (y_i - \bar{x}) \sin \omega t \right\}^2 \right]$$

$$= \frac{n}{2} (\tilde{A}^2 + \tilde{B}^2) = \frac{n}{2} \tilde{R}^2$$

in the three-parameter model.

2.3 LEAST SQUARES ESTIMATION OF FREQUENCY

In this section we show how the methods of Section 2.2 may be extended to include the estimation of the frequency ω . We shall deal only with the three-parameter "sinusoid plus constant" model, since that is the more generally useful. However, an exactly analogous method could be used to estimate ω in the two-parameter case. In the next section we shall extend the method further to the fitting of a number of frequencies (in fact, using the two-parameter method as the basic building block).

In Section 2.2 we found values $\hat{\mu}$, \hat{A} , and \hat{B} of μ , A , and B , respectively, to minimize

$$\begin{aligned} T(\mu, A, B) &= T(\mu, A, B, \omega) \\ &= \sum_{i=0}^{n-1} (x_i - \mu - A \cos \omega t - B \sin \omega t)^2, \end{aligned}$$

for a fixed ω . It was shown that these are approximately

$$\hat{\mu} = \bar{x} = \frac{1}{n} (x_0 + \cdots + x_{n-1}),$$

$$\hat{A}(\omega) = \frac{2}{n} \sum (x_i - \bar{x}) \cos \omega t,$$

$$\hat{B}(\omega) = \frac{2}{n} \sum (x_i - \bar{x}) \sin \omega t,$$

and furthermore that the residual sum of squares is

$$\begin{aligned} T\{\hat{\mu}(\omega), \hat{A}(\omega), \hat{B}(\omega), \omega\} &\approx T\{\bar{x}, \hat{A}(\omega), \hat{B}(\omega), \omega\} \\ &\approx T(\bar{x}, 0, 0, \omega) - \frac{n}{2} \{\hat{A}(\omega)^2 + \hat{B}(\omega)^2\} \\ &= T(\bar{x}, 0, 0, \omega) - \frac{n}{2} \tilde{R}(\omega)^2, \end{aligned}$$

where $\tilde{R}(\omega)^2 = \hat{A}(\omega)^2 + \hat{B}(\omega)^2$. In this section ω is regarded as an additional unknown, and so the dependence of the various estimates on ω is shown explicitly. The best value for ω in the sense of least squares is the value $\hat{\omega}$, that minimizes $T\{\hat{\mu}(\omega), \hat{A}(\omega), \hat{B}(\omega), \omega\}$. The corresponding approximation is the value $\tilde{\omega}$ that maximizes $\tilde{R}(\omega)^2$. Figure 2.1 shows a plot of part of the latter function for the variable-star data (Figure 1.1). An equivalent function used in later chapters is the *periodogram*

$$I(\omega) = \frac{n}{8\pi} \tilde{R}(\omega)^2.$$

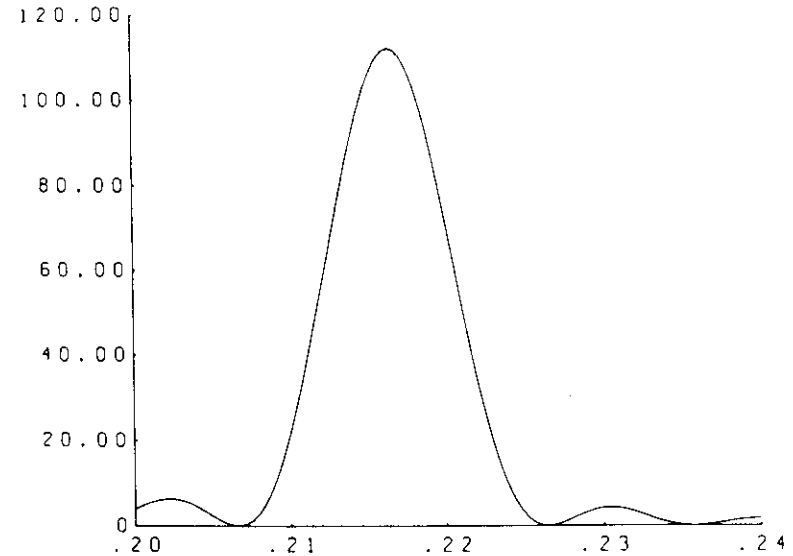


Figure 2.1 Periodogram of the variable-star data for frequencies ω , $0.20 < \omega < 0.24$.

Often, as in searching for a maximum or comparing function values, the actual values of the function are unimportant, and such rescalings have no impact. We shall therefore also refer to $\tilde{R}(\omega)^2$ as the periodogram when the difference is irrelevant.

The function

$$\frac{2}{n} [T(\bar{x}, 0, 0, \omega) - T\{\hat{\mu}(\omega), \hat{A}(\omega), \hat{B}(\omega), \omega\}]$$

was also calculated. However, it differed from $\tilde{R}(\omega)^2$ by at most 0.8, and hence it was not graphed. The graph shows a clear maximum at a value somewhat less than 0.220. The actual peak was found to be at $\omega = 0.21644$. The peak of the ungraphed function above was found to be at $\omega = 0.21641$. The difference is minor, especially since it is smaller than the difference between either value and the value found in Section 2.4. By contrast, the difference is appreciable in the light of the statistical results described in Section 2.6.

The least squares estimates of the parameters of a sinusoid with frequency $\omega = 0.21644$ are

$$\begin{aligned} \hat{\mu} &= 17.08, & \hat{A} &= 8.480, & \hat{B} &= 6.211, \\ \hat{\mu} = \bar{x} &= 17.11, & \tilde{A} &= 8.550, & \tilde{B} &= 6.225. \end{aligned}$$

The residual sum of squares for $\hat{\mu}$, \hat{A} , and \hat{B} is 14,977.2, while that for \bar{x} , \tilde{A} , and \tilde{B} is greater by 2.0, a negligible amount.

The graph also shows a subsidiary peak, or *sidelobe*, occurring on either side of the main peak, and separated from it by a trough in which the value is indistinguishable from zero. We shall see in Chapter 3 that this is typical of such graphs. The sidelobes do not indicate the presence of other periodicities.

The maxima of these functions were found numerically, using an algorithm described by Brent (1972). The derivatives of both functions with respect to ω are highly nonlinear and have many zeros (indeed, Figure 2.1 shows that there are six zeros just in the interval $0.20 \leq \omega \leq 0.24$). This makes an analytic solution impossible and also renders numerical methods based on the gradient treacherous. For instance, Newton's method could easily lead us to one of the other stationary points. (The FORTRAN program used is presented in the Appendix to this chapter.)

Figure 2.2 shows the residuals, that is, the original data less the fitted cosine term. They have a very pronounced periodicity with a period of around 24 days, or a frequency of approximately $\omega \approx 0.262$. Thus the original data must have contained at least these two periodic components. The estimation of a number of frequencies is described in the next section; in particular, we shall show that the presence of a second periodic component, especially one with a similar frequency, can noticeably distort the estimates of frequency and of amplitude and phase.

2.4 MULTIPLE PERIODICITIES

It emerged at the end of the preceding section that the data being used as an example actually contain more than one periodic component. In this section we describe how a number of components may be estimated, again using the variable-star data as an example.

The simplest procedure would be to repeat the analysis of Section 2.3, but searching now for a maximum near $\omega = 0.262$, the second frequency. If we distinguish quantities associated with the first (or second) frequency by the subscript 1 (or 2), we find that $\tilde{\omega}_2 = 0.2621$, $\tilde{A}_2 = -0.7579$, and $\tilde{B}_2 = 7.727$. However, the expressions for these estimates were obtained by the least squares fitting of the model

$$x_t = \mu + A \cos \omega t + B \sin \omega t + \epsilon_t,$$

where ϵ_t is the t th residual. The idea behind a least squares method is to make these residuals as small as possible. In the present case, however, the residual term necessarily includes the strong periodic component found in the preceding section, and it does not make sense to try to make this small.

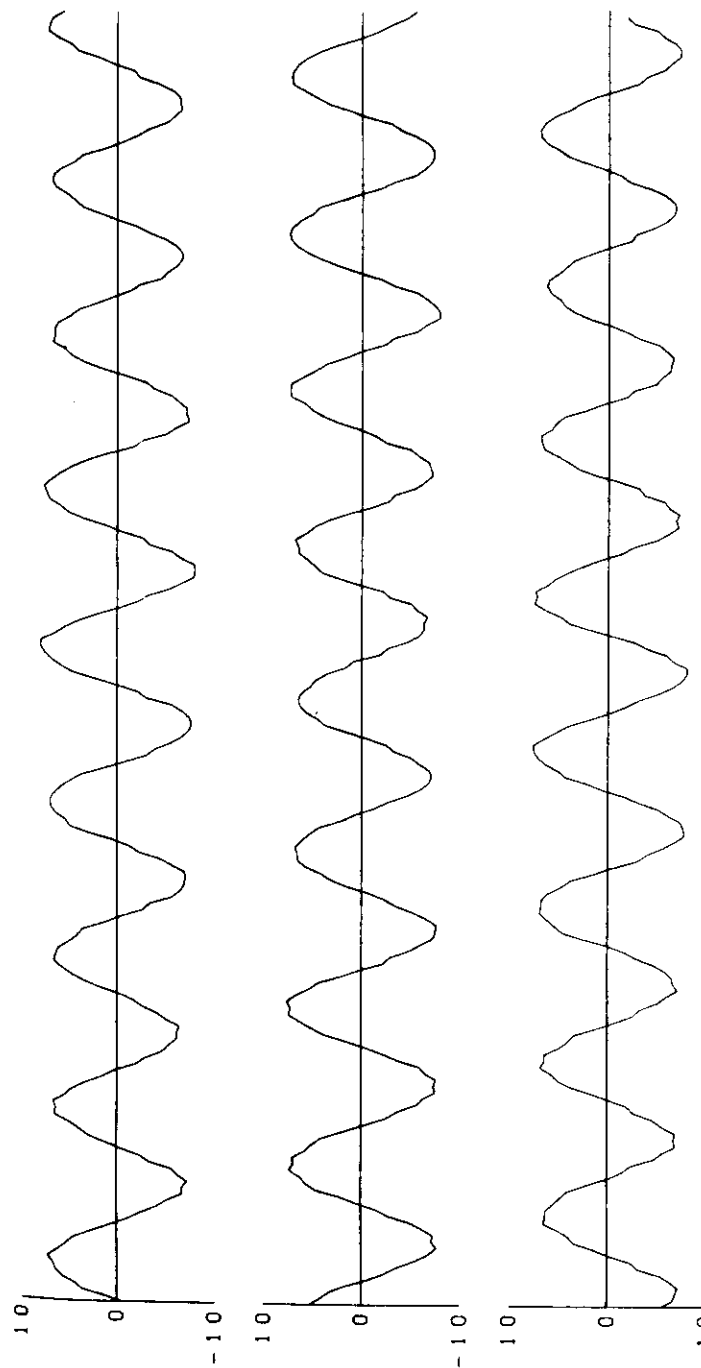


Figure 2.2 Variable-star data with fitted sinusoid subtracted.

A better approach is to include the second component in the model:

$$x_t = \mu + A_1 \cos \omega_1 t + B_1 \sin \omega_1 t + A_2 \cos \omega_2 t + B_2 \sin \omega_2 t + \varepsilon_t.$$

This leads us to minimize

$$\begin{aligned} \sum_{t=0}^{n-1} (x_t - \mu - A_1 \cos \omega_1 t - B_1 \sin \omega_1 t - A_2 \cos \omega_2 t - B_2 \sin \omega_2 t)^2 \\ = T(\mu, A_1, B_1, \omega_1, A_2, B_2, \omega_2), \quad \text{say.} \quad (6) \end{aligned}$$

The most natural extension of the method used in the Section 2.3 to find a single frequency is as follows. First, we note that for fixed ω_1 and ω_2 the model is linear in the remaining parameters. Hence the conditionally best values of these may be found by conventional methods and substituted in the function T (see Exercise 2.6). This gives us a new function

$$U(\omega_1, \omega_2) = T(\hat{\mu}, \hat{A}_1, \hat{B}_1, \omega_1, \hat{A}_2, \hat{B}_2, \omega_2),$$

where $\hat{\mu}$, \hat{A}_1 , \hat{B}_1 , and \hat{B}_2 are all functions of both ω_1 and ω_2 . The function U or an appropriate approximation could then be minimized numerically by one of the methods generally available (see Brent, 1972). Note that, by analogy with the functions examined in the preceding section, we can expect U to have many stationary points.

An alternative approach, which also builds on the method of Section 2.3 but avoids the explicit two-dimensional search, is based on the method of *cyclic descent*. The general idea of a cyclic descent method is to divide the parameters into subsets (exhaustive and usually exclusive), in such a way that the optimization with respect to parameters in any one subset, holding the remaining parameters fixed, can be done fairly easily. The method then is to update the subsets successively by solving these manageable optimization problems in turn. The basic method cycles through the subsets in some fixed order, until a complete cycle results in an effectively zero change in the function to be optimized. In sophisticated algorithms the subsets may be chosen in a different sequence so as to accelerate the convergence of the method, but we shall not do this. When the function cannot be reduced by varying any of the subsets of parameters, a (local) minimum has usually been reached. (For functions with continuous partial derivatives this is always the case, except for some pathological examples. However, the method can easily fail with functions that have discontinuous partial derivatives.)

For the sake of generality we shall describe a procedure using cyclic

descent to fit the more general model

$$x_t = \mu + \sum_{j=1}^m (A_j \cos \omega_j t + B_j \sin \omega_j t) + \varepsilon_t,$$

the model of "hidden periodicities," by least squares. First, minimization with respect to μ for fixed values of the other parameters is straightforward. The optimal value is just the mean of the "corrected" series

$$x_t - \sum_{j=1}^m (A_j \cos \omega_j t + B_j \sin \omega_j t), \quad t=0, \dots, n-1.$$

Next, if we vary ω_k , A_k , and B_k and hold the other parameters fixed, the problem is to minimize:

$$\begin{aligned} \sum_{t=0}^{n-1} \left\{ x_t - \mu - \sum_{\substack{j=1 \\ j \neq k}}^m (A_j \cos \omega_j t + B_j \sin \omega_j t) - A_k \cos \omega_k t - B_k \sin \omega_k t \right\}^2 \\ = \sum_{t=0}^{n-1} (y_t - A_k \cos \omega_k t - B_k \sin \omega_k t)^2, \end{aligned}$$

where

$$y_t = x_t - \mu - \sum_{j \neq k} (A_j \cos \omega_j t + B_j \sin \omega_j t).$$

The optimization with respect to ω_k , A_k , and B_k may be done as in Section 2.3, with the simplification that the single-frequency model does not include the added constant term.

Thus one cycle of the method consists of these two steps:

- (i) correct the data for all periodic components and estimate μ by the mean of the corrected series;
- (ii) for k running from 1 to m , correct the series for the mean μ and the other components; then estimate ω_k , A_k , and B_k from the corrected series.

A FORTRAN program based on this algorithm is presented in the Appendix to this chapter. It contains a switch (the logical variable APFLG) which allows one to select exact or approximate least squares for the single-frequency optimizations.

The results for the variable-star data are given in Table 2.1, together with the values found by the single-frequency method applied to the original data.

Note that the single-frequency estimates of frequency are very close to the values found by the cyclic descent method of this section. The sine and cosine coefficients are also similar, although not to the same extent. However, the residual sums of squares show that the cyclic descent estimates in fact provide a noticeably better fit to the data. Our conclusion is that, in the presence of strong components such as these, the single-frequency estimates do not give an adequate approximation to the least squares problem and are not satisfactory as estimates of the respective parameters. We could describe this by saying that the components *interfere* with each other. The interference is as strong as it is only because both components are strong and their frequencies are similar. A heuristic motivation for the cyclic descent method is that at each stage we remove all components other than the one currently being fitted, and thus avoid such interference.

Table 2.1 Different parameter estimates for the two-component model

| | Residual Sum of Squares | Component | Frequency | A | B |
|-------------------------|----------------------------|-----------|-----------|---------|--------|
| Method I ^a | 276.0 | 1 | 0.21644 | 8.5495 | 6.2108 |
| | | 2 | 0.26211 | -0.7579 | 7.7269 |
| Method II ^b | 59.6 | 1 | 0.21669 | 7.6551 | 6.5912 |
| | | 2 | 0.26172 | 0.1565 | 7.0828 |
| Method III ^c | 54.7 | 1 | 0.21666 | 7.6478 | 6.4905 |
| | | 2 | 0.26180 | 0.0006 | 7.0845 |

^aEstimating the two components separately from the original data.

^bCyclic descent method, approximate least squares.

^cCyclic descent method, exact least squares.

The reduction in the residual sum of squares to 54.7 is remarkable. The fact that the data were reported as integers means that they contain errors at least as large as that caused by rounding off a number to the nearest integer. Since the error incurred by such rounding off is roughly uniformly distributed from $-\frac{1}{2}$ to $\frac{1}{2}$, the mean squared error would be $\frac{1}{12}$. Thus from this cause alone we could expect a residual sum of squares of around

$600 \times \frac{1}{12} = 50$. Hence the unrounded data must have been almost exactly the sum of two pure sinusoids. A further curious feature of these data is that frequencies of 0.21669 and 0.26172 correspond to periods of 28.996 and 24.008 days, respectively, which are surprisingly close to integer values for the periods of a variable star.

Exercise 2.6 Least Squares Fitting with Fixed Frequencies

(i) The equations that result from equating the partial derivatives of (6) to zero are

$$-2 \sum_{t=0}^{n-1} (x_t - \mu - A_1 \cos \omega_1 t - B_1 \sin \omega_1 t - A_2 \cos \omega_2 t - B_2 \sin \omega_2 t) = 0,$$

$$-2 \sum_{t=0}^{n-1} \cos \omega_j t (x_t - \mu - A_1 \cos \omega_1 t - B_1 \sin \omega_1 t - A_2 \cos \omega_2 t - B_2 \sin \omega_2 t) = 0,$$

$$-2 \sum_{t=0}^{n-1} \sin \omega_j t (x_t - \mu - A_1 \cos \omega_1 t - B_1 \sin \omega_1 t - A_2 \cos \omega_2 t - B_2 \sin \omega_2 t) = 0,$$

$j = 1, 2$. Simplify these equations using the identities of Exercise 2.2, and show that they become diagonal if both frequencies are multiples of $2\pi/n$.

(ii) Show that if certain terms are ignored the last three equations become the same as those found in Section 2.2 for estimating the parameters of a single component of frequency ω , with $\omega = \omega_1$ and $\omega = \omega_2$, respectively. Obtain bounds for the errors introduced into the solution by this approximation.

(iii) Find bounds for the errors in the approximate solutions

$$\tilde{\mu} = \bar{x},$$

$$\tilde{A}_j = \frac{2}{n} \sum_{t=0}^{n-1} x_t \cos \omega_j t,$$

$$\tilde{B}_j = \frac{2}{n} \sum_{t=0}^{n-1} x_t \sin \omega_j t, \quad j = 1, 2.$$

2.5 THE EFFECT OF DISCRETE TIME: ALIASING

So far we have not discussed any restrictions that might need to be imposed on the frequency, ω , of the sinusoids being fitted to our data. Since the units of frequency are radians per unit time, it is natural to require that they be nonnegative. This may be justified by arguing that, since $\cos(-x) = \cos x$ and $\sin(-x) = -\sin x$, any cosine wave with negative frequency $-\omega$ can be written

$$A \cos(-\omega t) + B \sin(-\omega t) = A \cos \omega t + (-B) \sin \omega t,$$

as a cosine wave with a positive frequency. Thus the frequencies ω and $-\omega$ are indistinguishable; they are said to be *aliases* of each other.

The equal spacing in time of our observations introduces a further aliasing. Suppose that the *sampling interval* is Δ , so that the t th observation is made at time $t\Delta$. If the data consist of a pure cosine wave at frequency ω (for the sake of argument, with unit amplitude and zero phase), the t th observation will be

$$x_t = \cos \omega t \Delta.$$

If we increase ω from zero, this wave oscillates more and more rapidly until at $\omega = \pi/\Delta$ we have

$$x_t = \cos t\pi = (-1)^t,$$

which is clearly the most rapid oscillation we can observe. Suppose that we increase ω further, say to a value satisfying $\pi/\Delta < \omega < 2\pi/\Delta$. Let $\omega' = 2\pi/\Delta - \omega$. Then

$$\begin{aligned} x_t &= \cos \omega t \Delta \\ &= \cos \left(\frac{2\pi}{\Delta} - \omega' \right) t \Delta \\ &= \cos(2\pi t - \omega' t \Delta) \\ &= \cos \omega' t \Delta. \end{aligned}$$

In the same way $\sin \omega t \Delta = -\sin \omega' t \Delta$. Thus the frequencies ω and ω' are also indistinguishable and hence are aliases of each other. We may extend the argument to any positive frequency, no matter how large.

We conclude that every frequency not in the range $0 \leq \omega < \pi/\Delta$ has an alias in that range, termed its *principal alias*. To avoid indeterminacy, we shall restrict frequencies to this range. Figure 2.3 shows a number of

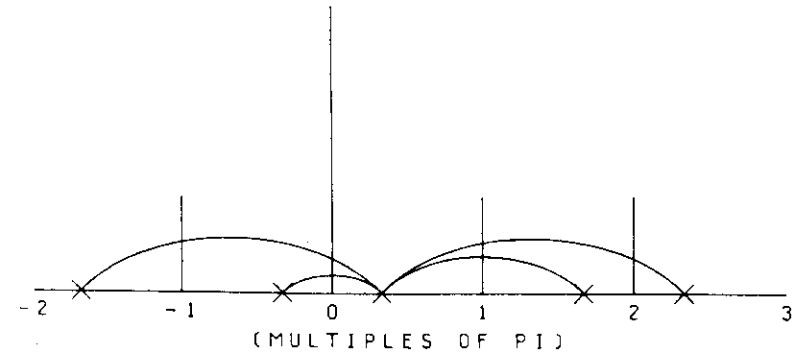


Figure 2.3 Some frequencies with the same principal alias.

frequencies with the same principal alias. The frequency π/Δ is known as the *Nyquist frequency*. It is also called the *folding frequency*, since effectively higher frequencies are folded down into the interval $[0, \pi/\Delta]$.

The Nyquist frequency is π/Δ in units of radians per unit time. In terms of cycles per unit time, it is therefore $1/(2\Delta)$. Since the sampling interval is Δ , the *sampling rate* is $1/\Delta$ observations per unit time. Thus the Nyquist frequency is one-half the sampling rate; in other words there are two samples per cycle of the Nyquist frequency, the highest frequency that can be observed.

The phenomenon of aliasing is important not only in the choice of frequencies to be fitted to data. It also must be borne in mind when designing a scheme to observe a time series. Suppose that $x(u)$ is a function of the continuous time parameter u , and that we wish to sample $x(u)$ to obtain information about frequencies in some interval, say (ω_0, ω_1) . Then usually we will want the Nyquist frequency to be greater than ω_1 so that all such frequencies are directly observable. However, if $x(u)$ contains oscillations with frequencies greater than ω_1 , we should choose the sampling frequency so that these are not aliased into the interval of interest. In fact, it is preferable when possible to remove these frequencies from the function before sampling, so that this problem cannot arise.

It should be noted that aliasing is a relatively simple phenomenon. In general, when one takes a discrete sequence of observations on a continuous function, information is lost. It is an advantage of the trigonometric functions that this loss of information is manifest in the easily understood form of aliasing.

In the chapters to follow, we shall often adopt the sampling interval as the unit of time. Then $\Delta = 1$, and the Nyquist frequency is simply π . Except where otherwise stated, this convention will be implicit.

2.6 SOME STATISTICAL RESULTS

In this chapter we have described how to obtain estimates of the coefficients of one or more sinusoidal components in a series. With the added assumption that the errors in the series are statistical or random in nature, we may describe the accuracy of those estimates.

Suppose that the data x_0, \dots, x_{n-1} were generated by the model

$$x_t = \mu + A \cos \omega t + B \sin \omega t + a_t, \quad (7)$$

where a_t are random errors or disturbances, and satisfy[†]

$$E(a_t) = 0,$$

$$E(a_t a_{t'}) = \begin{cases} v, & t = t' \\ 0, & \text{otherwise.} \end{cases}$$

The assumption that the errors at different times are uncorrelated is restrictive and is often violated in practice. We shall see in a later chapter how to make a more realistic assumption.

Having made statistical assumptions about the nature of the data, we may now make some statistical statements about the estimates discussed above. The exact least squares estimates \tilde{A} and \tilde{B} will not be considered. For the estimates \bar{x} , \tilde{A} , and \tilde{B} (of μ , A , and B , respectively) we can find exact expressions for the means, variances, and covariances. These are all lengthy expressions. However, it may be shown (see Exercises 2.7 to 2.9) that

$$E(\tilde{A}) \approx A, \quad E(\tilde{B}) \approx B, \quad E(\bar{x}) \approx \mu,$$

$$\text{var } \tilde{A} \approx \text{var } \tilde{B} \approx \frac{2v}{n}, \quad \text{var } \bar{x} \approx \frac{v}{n},$$

$$\text{corr}(\tilde{A}, \tilde{B}) \approx \text{corr}(\tilde{B}, \bar{x}) \approx \text{corr}(\bar{x}, \tilde{A}) \approx 0.$$

If we make the additional assumption that the errors a_0, \dots, a_{n-1} are independent, then by the central limit theorem (see, for instance, Feller, 1968, pp. 244, 254) we would expect \tilde{A} , \tilde{B} , and \bar{x} , as linear functions of the a 's, to be approximately normally distributed, with the stated means and variances. This may be verified by showing that the sequences of coefficients satisfy the relevant requirements.

The case in which ω is unknown and has to be estimated is more

[†]We use the conventional notation E to denote expectation.

difficult. It was first studied by Whittle (1952) and later by Walker (1971). The principal results for the estimate $\tilde{\omega}$ are that

$$E(\tilde{\omega}) = \omega + \text{terms involving } \frac{1}{n},$$

and

$$\text{var } \tilde{\omega} = \frac{24v}{n^3(A^2 + B^2)} + \text{smaller terms.}$$

At first sight, the n^{-3} behavior of $\text{var } \tilde{\omega}$ is surprising, since the variance of an estimated parameter usually behaves like the variances of \tilde{A} and \tilde{B} , that is, like n^{-1} . However, we may easily demonstrate that a higher power is appropriate.

Consider the case in which $R^2 = A^2 + B^2$ is large compared with v . Thus the data consist of clear oscillations, with small errors superimposed. Then we can count the number of cycles in our n data points accurately, and the only uncertainty involves the magnitude of the odd fraction of a period at each end of the data. If, for instance, we see m complete cycles, but not $m+1$, we can say that the period $2\pi/\omega$ lies between $n/(m+1)$ and n/m , or $2\pi m/n < \omega < 2\pi(m+1)/n$. Thus any estimate of ω should lie within $2\pi/n$ of the true value, and this implies that its variance is of order $1/n^2$ or better. The extra power of n is achieved by the relatively sophisticated estimate $\tilde{\omega}$.

The variance v of the errors is their mean square value. The corresponding quantity for the signal is

$$\begin{aligned} \text{ave}(A \cos \omega t + B \sin \omega t)^2 &= \text{ave}\{R \cos(\omega t + \phi)\}^2 \\ &= R^2 \text{ave} \cos^2(\omega t + \phi) \\ &= \frac{R^2}{2}. \end{aligned}$$

The quantity

$$\frac{R^2/2}{v} = \frac{\text{mean square value of signal}}{\text{mean square value of noise}},$$

called the *signal-to-noise ratio* or *snr*, indicates how well the signal shows up in the noise. The variance of $\tilde{\omega}$ may be rewritten as

$$\text{var } \tilde{\omega} \approx \frac{12}{n^3 \text{snr}},$$

which shows, somewhat surprisingly, that a long series is more important than a strong signal.

For the variable-star data, these formulas yield standard deviations for the two frequencies of 1.04×10^{-5} (for frequency 0.2167) and 1.49×10^{-5} (for frequency 0.2618). These values show that the frequencies are in theory capable of very sharp resolution. It should be noted, however, that this result depends heavily on the assumptions made, especially independence of the errors.

The variances of \tilde{A} and \tilde{B} are increased by replacing ω by its estimate $\tilde{\omega}$. The results are

$$\text{var } \tilde{A} \approx \frac{2v}{n} \frac{A^2 + 4B^2}{R^2},$$

$$\text{var } \tilde{B} \approx \frac{2v}{n} \frac{4A^2 + B^2}{R^2},$$

$$\text{cov}(\tilde{A}, \tilde{B}) \approx \frac{6v}{n} \frac{AB}{R^2},$$

$$\text{cov}(\tilde{A}, \tilde{\omega}) \approx \frac{12v}{n^2} \frac{B}{R^2},$$

$$\text{cov}(\tilde{B}, \tilde{\omega}) \approx \frac{-12v}{n^2} \frac{A}{R^2}.$$

Furthermore, estimates concerning different frequencies are, to this order of approximation, uncorrelated. Since, as Walker shows, \tilde{A} , \tilde{B} , and $\tilde{\omega}$ are all approximately normally distributed, these results allow us to find confidence intervals for the corresponding parameters.

In the light of the (approximate) standard deviations of the two estimated frequencies, it is instructive to recall that their final estimates differed by many times these quantities from the first values, computed directly from the data containing both components (see Table 2.1). Since the two frequencies are fairly close, they interact or interfere with each other, and this effect dominates the statistical error, unless it is removed, as in the simultaneous estimation procedure of Section 2.4. Pisarenko (1973) has shown that when a series contains two very similar frequencies the above formulas for variances and covariances may not be valid. Although Pisarenko's results are for frequencies closer than those in the present data, they suggest that we should treat the standard deviations given above with some caution.

Exercise 2.7 The Estimates \bar{x} , \tilde{A} , and \tilde{B}

Suppose that the data $\{x_0, \dots, x_{n-1}\}$ were generated by the model (7). Show that

$$\bar{x} = \mu + \bar{a} + \left\{ A \cos \frac{(n-1)\omega}{2} + B \sin \frac{(n-1)\omega}{2} \right\} D_n(\omega),$$

where

$$D_n(\omega) = \frac{\sin n\omega/2}{n \sin \omega/2}.$$

Show also that

$$\begin{aligned} \tilde{A} = A + \frac{2}{n} \sum a_i \cos \omega i + \{ A \cos(n-1)\omega + B \sin(n-1)\omega \} D_n(2\omega) \\ - 2\bar{a} \cos \frac{(n-1)\omega}{2} D_n(\omega), \end{aligned}$$

$$\begin{aligned} \tilde{B} = B + \frac{2}{n} \sum a_i \sin \omega i + \{ A \sin(n-1)\omega + B \cos(n-1)\omega \} D_n(2\omega) \\ - 2\bar{a} \sin \frac{(n-1)\omega}{2} D_n(\omega). \end{aligned}$$

Exercise 2.8 Continuation

The bias of \bar{x} as an estimator of μ is

$$b = \left\{ A \cos \frac{(n-1)\omega}{2} + B \sin \frac{(n-1)\omega}{2} \right\} D_n(\omega),$$

since $E\bar{a} = 0$. Show that

$$|b| \leq \frac{R}{n \sin \omega/2},$$

where, as usual, $R^2 = A^2 + B^2$. Find the bias of \tilde{A} and show that it may similarly be bounded by

$$\frac{R}{n} \left\{ \frac{1}{\sin \omega} + \frac{2}{n(\sin \omega/2)^2} \right\} + \frac{2\mu}{n \sin \omega/2}.$$

Show that the same quantity is a bound for the bias of \tilde{B} .

Exercise 2.9 Continuation

Show that the variance of \bar{x} is v/n , and that the variances of \tilde{A} and \tilde{B} differ from $2v/n$ by, at most, $(2v/n)/(n\sin\omega)$. Find the covariance of A and B , and show that it too is bounded by this same quantity.

Show that the covariances of \bar{x} with \tilde{A} and \tilde{B} are both bounded by $(2v/n)/(n\sin\omega/2)$.

APPENDIX

The following program was used to fit the two-component model discussed in Section 2.4 and may also serve to fit the more general m -component model. Subprograms OPTOM, LOCALM, SSREG, STATS, and PARMS carry out the actual fitting algorithm. The main program and the subroutine DATIN are used solely for input/output.

These programs may also be used to fit the single-frequency model of Section 2.3, as a special case of the general model. The exact least squares method is found by setting APPFLG to .FALSE., and LIM and CONV to values that allow the algorithm to iterate to convergence (say, $\text{CONV} = 1\text{E}-5$ and $\text{LIM} = 5$). The approximate method is used by setting APPFLG to .TRUE., and LIM and CONV so that only one cycle is performed (that is, $\text{LIM} = 1$ or CONV set to a relatively large value, say π).

NOTE: If any frequency is initialized at a value outside the range $[0, \pi]$, the final value will likewise fail to be its principal alias.

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NOTE: If any frequency is initialized at a value outside the range $[0, \pi]$, the final value will likewise fail to be its principal alias.

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```

C
C THIS MAIN PROGRAM AND SUBROUTINE DATIN ARE USED TO
C INPUT DATA FOR, AND OUTPUT RESULTS FROM, FITTING A
C MODEL OF HIDDEN PERIODICITIES TO A TIME SERIES.
C THE TIME SERIES DATA COME FIRST IN THE INPUT FILE.
C (FOR THE FORMAT SEE DATIN.) THE FIRST CARD AFTER THE
C TIME SERIES CONTAINS THE VALUES OF THE VARIABLES
C CONV, LIM AND APPFLG, WHICH CONTROL THE OPERATION
C OF THE FITTING ALGORITHM, IN F10.5,15,L1 FORMAT.
C NEXT COMES A CARD WITH THE NUMBER OF COMPONENTS, IN
C I5 FORMAT.
C FOLLOWING THIS, THERE IS ONE CARD FOR EACH FREQUENCY
C TO BE FITTED. IT CONTAINS THE STARTING VALUES OF THE
C FREQUENCY AND THE COSINE AND SINE COEFFICIENTS, IN
C 3F10.5 FORMAT.
C
      DIMENSION X(600),FRE(10),A(10),B(10)
      LOGICAL APPFLG
      CALL DATIN (X,N,START,STEP,5)
      READ (5,1) CONV,LIM,APPFLG
1     FORMAT (F10.5,15,L1)
      WRITE(6,4) CONV,LIM,APPFLG
4     FORMAT ('#FOR THIS RUN, CONV =*,E12.4/
      +      * LIM =*,I5/
      +      * APPFLG =*,L5)
      READ(5,8) M
8     FORMAT(15)
      DO 10 J=1,M
10    READ (5,2) FRE(J),A(J),B(J)
2     FORMAT (3F10.5)
      WRITE(6,5)
5     FORMAT('#0INITIAL VALUES ARE -*)
      WRITE(6,3) (J,FRE(J),A(J),B(J),J=1,M)
3     FORMAT(* COMPONENT FREQUENCY      COSINE      SINE*/
      +      * CUEFFICIENTS*/
      +      (15,F15.7,2E15.6))
      CALL OPTOM (X,N,RMU,FRE,A,B,M,CONV,LIM,APPFLG)
      WRITE(6,6)
6     FORMAT('#0 FINAL VALUES ARE -*)
      WRITE(6,3) (IM,FRE(IM),A(IM),B(IM),IM=1,M)
      SS=0.0
      DO 30 I=1,N
      TEMP=X(I)-RMU
      DO 40 J=1,M
      ARG=FLOAT(I-1)*FRE(J)
      TEMP=TEMP-A(J)*COS(ARG)-B(J)*SIN(ARG)
40    CONTINUE
      SS=SS+TEMP**2
30    CONTINUE
      WRITE(6,7) RMU,SS
7     FORMAT('#0FITTED CONSTANT IS      *,E15.5/
      +      * RESIDUAL SUM OF SQUARES IS*,E15.6)
      STOP
      END

```

```

C      SUBROUTINE DATIN (X,N,START,STEP,M)
C      THIS SUBROUTINE IS USED TO INPUT A SERIES OF VALUES
C      (IN RUN-TIME FORMAT) AND SOME ASSOCIATED QUANTITIES
C      (IN FIXED FORMAT). THE FIRST FOUR DATA CARDS ARE -
C      1 A HEADER CARD (72 COLUMNS)
C      2 VALUE OF N (15)
C      3 THE DATA FORMAT (72 COLUMNS)
C      4 START AND STEP (2F10.5)
C      PARAMETERS ARE -
C
C      NAME      TYPE      ON ENTRY      VALUE      ON RETURN
C
C      X      REAL ARRAY NOT USED      THE SERIES
C      N      INTEGER      NOT USED      SERIES LENGTH
C      START REAL      NOT USED      TIME VALUE AT THE
C                                     FIRST DATA POINT
C      STEP  REAL      NOT USED      TIME INCREMENT
C                                     BETWEEN DATA POINTS
C      M      INTEGER      LOGICAL UNIT NUMBER      UNCHANGED
C
C      DIMENSION X(600),HEAD(18),FMT(18)
C      READ(M,1) HEAD,N,FMT,START,STEP
C      FORMAT(18A4/15/18A4/2F10.5)
C      WRITE(6,2) HEAD,N,FMT,START,STEP
C      2      FORMAT(*GTHE DATA HEADER READS -*/1X,18A4/
C      +          * THE SERIES LENGTH IS*,I6/
C      +          * THE DATA FORMAT IS -*/1X,18A4/
C      +          * TIME ORIGIN IS*,F11.5,
C      +          *, TIME INCREMENT IS*,F11.5)
C      READ(M,FMT) (X(I),I=1,N)
C      RETURN
C      END

```

```

C      SUBROUTINE OPTOM (X,N,RMU,FRE,A,B,M,CONV,LIM,APPLG)
C      THIS SUBROUTINE, WITH SUBPROGRAMS LOCALM, SSREG,
C      STATS AND PARMS, IMPLEMENTS THE ALGORITHM
C      FOR THE LEAST-SQUARES FITTING OF THE
C      MODEL OF HIDDEN PERIODICITIES. PARAMETERS ARE
C
C      NAME      TYPE      ON ENTRY      VALUE      ON RETURN
C
C      X      REAL ARRAY THE TIME SERIES      UNCHANGED
C      N      INTEGER      SERIES LENGTH      UNCHANGED
C      RMU     REAL      NOT USED      CONSTANT TERM
C      FRE     REAL ARRAY STARTING VALUES FOR      FINAL VALUES
C                                     THE FREQUENCIES TO
C                                     BE FITTED
C      A      REAL ARRAY STARTING VALUES FOR      FINAL VALUES
C                                     COSINE COEFFICIENTS
C      B      REAL ARRAY STARTING VALUES FOR      FINAL VALUES
C                                     SINE COEFFICIENTS
C      M      INTEGER      NUMBER OF COMPONENTS      UNCHANGED
C                                     TO BE FITTED
C      CONV    REAL      CONVERGENCE CRITERION      UNCHANGED
C                                     ITERATION CEASES WHEN
C                                     IN ONE CYCLE, NO
C                                     FREQUENCY CHANGES BY
C                                     MORE THAN CONV
C      LIM     INTEGER      MAXIMUM NUMBER OF      UNCHANGED
C                                     CYCLES OF ITERATION
C      APPLG   LOGICAL      FLAG CONTROLLING      UNCHANGED
C                                     WHETHER APPROXIMATE
C                                     (.TRUE.) OR EXACT
C                                     (.FALSE.) LEAST SQUARES
C                                     IS TO BE USED

```

C NOTES.
 C 1. IF VALUES OF N OR M EXCEEDING 600 AND 10,
 C RESPECTIVELY, ARE USED, THE DIMENSION
 C STATEMENT BELOW SHOULD BE CHANGED ACCORDINGLY.
 C 2. USE OF EXACT LEAST SQUARES (APPFLG = .FALSE.)
 C WILL CAUSE LONGER EXECUTION TIMES.
 C 3. THE FREQUENCIES IN GENERAL CONVERGE TO VALUES
 C WITHIN $2\pi/N$ OF THEIR STARTING VALUES. THE
 C STARTING VALUES SHOULD BE GIVEN TO AT LEAST THIS
 C ACCURACY, OR THE ALGORITHM MAY BE TRAPPED BY
 C SIDE-LOBES. STARTING VALUES OF THE COSINE AND
 C SINE COEFFICIENTS ARE LESS CRITICAL, AND MAY BE
 C SET TO ZERO.

```

C REAL LOCALM
C DIMENSION X(N),Y(600),FRE(10),A(10),B(10)
C LOGICAL APPFLG
C DATA EPS /1E-9/
C T=CONV
C DELTA =3.142/FLOAT(N)
C DO 10 KOUNT=1,LIM
C SUM=0
C DO 20 I=1,N
C Y(I)=X(I)
C DO 30 J=1,M
C ARG=FLOAT(I-1)*FRE(J)
C Y(I)=Y(I)-(J)*COS(ARG)-B(J)*SIN(ARG)
30 SUM=SUM+Y(I)
20 SUM=SUM+Y(I)
C RMU=SUM/FLOAT(N)
C TEST=0
C DO 40 J=1,M
C DO 50 I=1,N
C Y(I)=X(I)-RMU
C DO 50 K=1,M
C IF(K .EQ. J) GO TO 50
C ARG=FLOAT(I-1)*FRE(K)
C Y(I)=Y(I)-A(K)*COS(ARG)-B(K)*SIN(ARG)
50 CONTINUE
C DUMMY=LOCALM (FRE(J)-DELTA,FRE(J)+DELTA,
C EPS,T,TEMP,Y,N,APPFLG)
C TEST=AMAX1(TEST,ABS(FRE(J)-TEMP))
C FRE(J)=TEMP
C CALL PARMS (Y,N,FRE(J),APPFLG,A(J),B(J))
C IF (TEST .LT. CONV) RETURN
C DELTA=TEST+2.0*T
10 CONTINUE
C RETURN
C END
  
```

```

C REAL FUNCTION LOCALM (A,B,EPS,T ,X,Y,N,APPFLG)
C REAL FUNCTION LOCALM (A,B,EPS,T,F,X)
C THIS IS THE FORTRAN FUNCTION LOCALM GIVEN BY
C RICHARD BRENT IN
C ALGORITHMS FOR MINIMIZATION WITHOUT DERIVATIVES,
C (PRENTICE-HALL, 1973).
C IT FINDS A LOCAL MINIMUM OF THE FUNCTION F IN THE
C INTERVAL (A,B).
C T AND EPS DEFINE A TOLERANCE TOL = EPS*ABS(X)+T,
C WHERE X IS THE CURRENT APPROXIMATION TO THE POSITION
C OF THE MINIMUM. THE MINIMUM IS FOUND WITH AN ERROR
C OF AT MOST 3*TOL.
C F IS NOT EVALUATED AT POINTS CLOSER THAN TOL.
C A SUITABLE VALUE FOR EPS IS THE SQUARE ROOT OF THE
C RELATIVE MACHINE PRECISION. FOR MORE DETAILS SEE THE
C ABOVE REFERENCE.
C
C DIMENSION Y(N)
C REAL M
C SA=A
C SB=B
C X=SA+0.381966*(SB-SA)
C W=X
C V=W
C E=0.0
C FX=F(X)
C C FX=-SSREG(Y,N,X,APPFLG)
C FW=FX
C FV=FV
10 M=0.5*(SA+SB)
C TOL=EPS*ABS(X)+T
C T2=2.0*TOL
C IF(ABS(X-M) .LE. T2-0.5*(SB-SA)) GO TO 190
C R=0.0
C Q=R
C P=Q
C IF (ABS(E) .LE. TOL) GO TO 40
C R=(X-W)*(FX-FV)
C Q=(X-V)*(FX-FW)
C P=(X-V)*Q-(X-W)*R
C Q=2.0*(Q-R)
C IF (Q .LE. 0.0) GO TO 20
C P=-P
C GO TO 30
20 Q=-Q
30 R=E
C E=D
40 IF (ABS(P) .GE. ABS(0.5*Q*R)) GO TO 60
C IF ((P .LE. Q*(SA-X)) .OR. (P .GE. Q*(SB-X))) GO TO 60
C D=P/Q
C U=X+D
C IF((U-SA .GE. T2) .AND. (SB-U .GE. T2)) GO TO 90
C IF (X .GE. M) GO TO 50
C D=TOL
  
```

```

      GO TO 90
50    D=-TOL
      GO TO 90
60    IF (X .GE. M) GO TO 70
      E=SB-X
      GO TO 80
70    E=SA-X
80    D=0.381966*E
90    IF (ABS(D) .LT. TOL) GO TO 100
      U=X+D
      GO TO 120
100   IF (D .LE. 0.0) GO TO 110
      U=X+TOL
      GO TO 120
110   U=X-TOL
C120  FU=F(U)
120   FU=-SSREG(Y,N,U,APPFLG)
      IF (FU .GT. FX) GO TO 150
      IF (U .GE. X) GO TO 130
      SB=X
      GO TO 140
130   SA=X
140   V=W
      FV=FW
      W=X
      FW=FX
      X=U
      FX=FU
      GO TO 10
150   IF (U .GE. X) GO TO 160
      SA=U
      GO TO 170
160   SB=U
170   IF ((FU .GT. FW) .AND. (W .NE. X)) GO TO 180
      V=W
      FV=FW
      W=U
      FW=FU
      GO TO 10
180   IF ((FU .GT. FV) .AND. (V .NE. X) .AND. (V .NE. W))
+     GO TO 10
      V=U
      FV=FU
      GO TO 10
190   LOCALM=FX
      RETURN
      END

```

```

      FUNCTION SSREG (Y,N,OMEGA,APPFLG)
C
C   THIS FUNCTION RETURNS THE SUM OF SQUARES (APPROXIMATE
C   OR EXACT) ASSOCIATED WITH OMEGA. PARAMETERS ARE
C
C   NAME      TYPE      VALUE ON ENTRY (NONE ARE CHANGED)
C
C   Y         REAL ARRAY THE TIME SERIES
C
C   N         INTEGER    SERIES LENGTH
C
C   OMEGA     REAL       THE FREQUENCY
C
C   APPFLG    LOGICAL    .TRUE. FOR APPROXIMATE LEAST SQUARES,
C                        .FALSE. FOR EXACT LEAST SQUARES
C
      DIMENSION Y(N)
      LOGICAL APPFLG
      CALL STATS (Y,N,OMEGA,CY,SY)
      IF (APPFLG) GO TO 10
      RN=N
      CON=SIN(RN*OMEGA)/SIN(OMEGA)
      ARG=(RN-1.0)*OMEGA
      CC=0.5*(RN+COS(ARG)*CON)
      CS=0.5*SIN(ARG)*CON
      SS=RN-CC
      SSREG=(SS*CY**2-2.0*CS*CY*SY+CC*SY**2)/(CC*SS-CS**2)
      RETURN
10    CONTINUE
      SSREG=(CY**2+SY**2)*2.0/FLOAT(N)
      RETURN
      END

```

```

C      SUBROUTINE STATS (Y,N,OMEGA,CY,SY)
C      THIS SUBROUTINE RETURNS THE COSINE AND SINE SUMS OF A
C      TIME SERIES.  PARAMETERS ARE
C      NAME      TYPE      ON ENTRY      VALUE      ON RETURN
C      Y      REAL ARRAY THE TIME SERIES      UNCHANGED
C      N      INTEGER      SERIES LENGTH      UNCHANGED
C      OMEGA REAL      THE FREQUENCY      UNCHANGED
C      CY      REAL      NOT USED      COSINE SUM
C      SY      REAL      NOT USED      SINE SUM
C      DIMENSION Y(N)
C      CY=0.0
C      SY=0.0
C      DO 10 I=1,N
C      ARG=FLOAT(I-1)*OMEGA
C      CY=CY+COS(ARG)*Y(I)
C      SY=SY+SIN(ARG)*Y(I)
10  CONTINUE
C      RETURN
C      END

```

```

C      SUBROUTINE PARMS (Y,N,OMEGA,APPFLG,A,B)
C      THIS SUBROUTINE RETURNS THE (EXACT OR APPROXIMATE)
C      LEAST SQUARES ESTIMATES OF THE COSINE AND SINE
C      COEFFICIENTS OF A SINGLE PERIODIC COMPONENT.
C      PARAMETERS ARE
C      NAME      TYPE      ON ENTRY      VALUE      ON RETURN
C      Y      REAL ARRAY THE TIME SERIES      UNCHANGED
C      N      INTEGER      SERIES LENGTH      UNCHANGED
C      OMEGA REAL      THE FREQUENCY      UNCHANGED
C      APPFLG LOGICAL      .TRUE. OR .FALSE.      UNCHANGED
C      FOR APPROXIMATE OR
C      EXACT LEAST SQUARES,
C      RESPECTIVELY
C      A      REAL      NOT USED      COS COEFFICIENT
C      B      REAL      NOT USED      SIN COEFFICIENT
C      LOGICAL APPFLG
C      DIMENSION Y(N)
C      CALL STATS (Y,N,OMEGA,CY,SY)
C      RN=FLOAT(N)
C      IF (SIN(OMEGA) .EQ. 0.0) GO TO 20
C      IF (APPFLG) GO TO 10
C      CON=SIN(RN*OMEGA)/SIN(OMEGA)
C      ARG=(RN-1.0)*OMEGA
C      CC=0.5*(RN+COS(ARG)*CON)
C      CS=0.5*SIN(ARG)*CON
C      SS=RN-CC
C      DEL=CC*SS-CS**2
C      A=(CY*SS-SY*CS)/DEL
C      B=(SY*CC-CY*CS)/DEL
C      RETURN
10  CONTINUE
C      A=2.0*CY/RN
C      B=2.0*SY/RN
C      RETURN
20  A=CY/RN
C      B=0.0
C      RETURN
C      END

```