CHAPTER 24

An Introduction to Nonlinear Estimation

24.1. LEAST SQUARES FOR NONLINEAR MODELS

Introduction

This chapter introduces nonlinear estimation, which involves the fitting of nonlinear models by least squares. The normal equations are not linear in this application and are, in general, difficult to solve. Direct minimization of the sum of squares function is usually performed. This typically requires heavy iterative calculations and the use of a special program. Although the details and outputs of such programs vary, the basic material in this chapter applies whichever program the reader selects. The exercises (and their solutions) provide a variety of examples of nonlinear data and the models fitted to them.

Nonlinear Models

In previous chapters we have mostly fitted, by least squares, models that were *linear in the parameters* and were of the type

$$Y = \beta_0 + \beta_1 Z_1 + \beta_2 Z_2 + \cdots + \beta_{p-1} Z_{p-1} + \epsilon, \tag{24.1.1}$$

where the Z_i can represent any functions of the basic predictor variables $X_1, X_2, \ldots, X_k$. While Eq. (24.1.1) can represent a wide variety of relationships, there are many situations in which a model of this form is not appropriate; for example, when definite information is available about the form of the relationship between the response and the predictor variables. Such information might involve direct knowledge of the actual form of the true model or might be represented by a set of differential equations that the model must satisfy. Sometimes the information leads to several alternative models (in which case methods for discriminating between them will be of interest). When we are led to a model of nonlinear form, we would usually prefer to fit such a model whenever possible, rather than to fit an alternative, perhaps less realistic, linear model.

Any model that is *not* of the form given in Eq. (24.1.1) will be called a *nonlinear model,* that is, nonlinear in the *parameters.* Two examples of such models are

$$Y = \exp(\theta_1 + \theta_2 t + \epsilon), \tag{24.1.2}$$

$$Y = \frac{\theta_1}{\theta_1 - \theta_2}[e^{-\theta_2 t} - e^{-\theta_1 t}] + \epsilon. \tag{24.1.3}$$

In these examples the parameters to be estimated are denoted by θ's rather than β's as used previously, t is the single predictor variable, and ϵ is a random error term with $E(\epsilon) = 0$, $V(\epsilon) = \sigma^2$. (We could also write these models without ϵ and replacing Y by η. Then, the models would show how *true* values of the response, η, depend on t. Here, we wish to be specific about how the error enters the model to permit the discussion that follows.)

The models in Eqs. (24.1.2) and (24.1.3) are both nonlinear in the sense that they involve θ_1 and θ_2 in a nonlinear way but they are of essentially different characters. Equation (24.1.2) can be transformed, by taking logarithms to the base e, into the form

$$\ln Y = \theta_1 + \theta_2 t + \epsilon, \tag{24.1.4}$$

which is the form of Eq. (24.1.1) and is *linear* in the parameters. We can thus say that the model given in Eq. (24.1.2) is *intrinsically linear* since it can be transformed into linear form. (Some writers use the phrase *nonintrinsically nonlinear,* but we shall not.)

However, it is impossible to convert Eq. (24.1.3) into a form linear in the parameters. Such a model is said to be *intrinsically nonlinear.* While, at times, it may be useful to transform a model of this type so that it can be more easily fitted, it will remain a nonlinear model, whatever the transformation applied. Unless specifically noted, all models mentioned in this chapter will be intrinsically nonlinear.

Note: In models in which the error is additive, an intrinsically linear model is one that can be made linear by a transformation of parameters; for example, $Y = e^{\theta}X + \epsilon$ is of this type since, if we transform by $\beta = e^{\theta}$, the model becomes $Y = \beta X + \epsilon$. Other authors use the words *intrinsically linear* in this sense only.

Least Squares in the Nonlinear Case

The standard notation for nonlinear least squares situations is different from that for linear least squares cases. This may seem confusing to the reader at first, but the notation is well established in the literature. The differences are shown in Table 24.1.

Suppose the postulated model is of the form

$$Y = f(\xi_1, \xi_2, \ldots, \xi_k; \theta_1, \theta_2, \ldots, \theta_p) + \epsilon. \tag{24.1.5}$$

If we write

$$\boldsymbol{\xi} = (\xi_1, \xi_2, \ldots, \xi_k)',$$
$$\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_p)',$$

T A B L E 24.1. Standard Notations for Linear and Nonlinear Least Squares

	Linear	Nonlinear
Response	Y	Y
Subscripts of observations	$i = 1, 2, \ldots, n$	$u = 1, 2, \ldots, n$
Predictor variables	$X_1, X_2, \ldots, X_k$	$\xi_1, \xi_2, \ldots, \xi_k$ (Sometimes t = time, or T = temperature, etc., sometimes even $X_1, X_2, \ldots, X_k$)
Parameters	$\beta_0, \beta_1, \ldots, \beta_p$	$\theta_0, \theta_1, \ldots, \theta_p$ (Sometimes, $\alpha, \beta, \ldots, \phi, \ldots$, etc.)

we can shorten Eq. (24.1.5) to

$$Y = f(\boldsymbol{\xi}, \boldsymbol{\theta}) + \epsilon$$

or

$$E(Y) = f(\boldsymbol{\xi}, \boldsymbol{\theta}) \tag{24.1.6}$$

if we assume that $E(\epsilon) = 0$. We shall also assume that errors are uncorrelated, that $V(\epsilon) = \sigma^2$, and, usually, that $\epsilon \sim N(0, \sigma^2)$ so that errors are independent.

When there are n observations of the form

$$Y_u, \xi_{1u}, \xi_{2u}, \ldots, \xi_{ku},$$

for $u = 1, 2, \ldots, n$, available, we can write the model in the alternative form

$$Y_u = f(\xi_{1u}, \xi_{2u}, \ldots, \xi_{ku}; \theta_1, \theta_2, \ldots, \theta_p) + \epsilon_u, \tag{24.1.7}$$

where ϵ_u is the uth error, $u = 1, 2, \ldots, n$. This can be abbreviated to

$$Y_u = f(\boldsymbol{\xi}_u, \boldsymbol{\theta}) + \epsilon_u, \tag{24.1.8}$$

where $\boldsymbol{\xi}_u = (\xi_{1u}, \xi_{2u}, \ldots, \xi_{ku})'$. The assumption of normality and independence of the errors can now be written as $\boldsymbol{\epsilon} \sim N(\mathbf{0}, \mathbf{I}\sigma^2)$, where $\boldsymbol{\epsilon} = (\epsilon_1, \epsilon_2, \ldots, \epsilon_n)'$, and as usual $\mathbf{0}$ is a vector of zeros and $\mathbf{I}$ is a unit matrix, both of appropriate sizes. We define the *error sum of squares* for the nonlinear model and the given data as

$$S(\boldsymbol{\theta}) = \sum_{u=1}^{n} \{Y_u - f(\boldsymbol{\xi}_u, \boldsymbol{\theta})\}^2. \tag{24.1.9}$$

Note that since Y_u and $\boldsymbol{\xi}_u$ are fixed observations, the sum of squares is a function of $\boldsymbol{\theta}$. We shall denote by $\hat{\boldsymbol{\theta}}$, a *least squares esimate* of $\boldsymbol{\theta}$, that is a value of $\boldsymbol{\theta}$ which minimizes $S(\boldsymbol{\theta})$. [It can be shown that, if $\boldsymbol{\epsilon} \sim N(\mathbf{0}, \mathbf{I}\sigma^2)$, the least squares estimate of $\boldsymbol{\theta}$ is also the maximum likelihood estimate of $\boldsymbol{\theta}$. This is because the likelihood function for this problem can be written

$$\ell(\boldsymbol{\theta}, \sigma^2) = (2\pi\sigma^2)^{-n/2} e^{-S(\boldsymbol{\theta})/2\sigma^2}$$

so that if σ^2 is known, maximizing $\ell(\boldsymbol{\theta}, \sigma^2)$ with respect to $\boldsymbol{\theta}$ is equivalent to minimizing $S(\boldsymbol{\theta})$ with respect to $\boldsymbol{\theta}$.]

To find the least squares estimate $\hat{\boldsymbol{\theta}}$ we need to differentiate Eq. (24.1.9) with respect to $\boldsymbol{\theta}$. This provides the p *normal equations,* which must be solved for $\hat{\boldsymbol{\theta}}$. The normal equations take the form

$$\sum_{u=1}^{n} \{Y_u - f(\boldsymbol{\xi}_u, \hat{\boldsymbol{\theta}})\} \left[\frac{\partial f(\boldsymbol{\xi}_u, \boldsymbol{\theta})}{\partial \theta_i} \right]_{\boldsymbol{\theta} = \hat{\boldsymbol{\theta}}} = 0 \tag{24.1.10}$$

for $i = 1, 2, \ldots, p$, where the quantity denoted by brackets is the derivative of $f(\boldsymbol{\xi}_u, \boldsymbol{\theta})$ with respect to θ_i with all θ's replaced by the corresponding $\hat{\theta}$'s, which have the same subscript. We recall that when the function $f(\boldsymbol{\xi}_u, \boldsymbol{\theta})$ was linear this quantity was a function of the $\boldsymbol{\xi}_u$ only and did not involve the $\hat{\theta}$'s at all. For example, if

$$f(\boldsymbol{\xi}_u, \boldsymbol{\theta}) = \theta_1 \xi_{1u} + \theta_2 \xi_{2u} + \cdots + \theta_p \xi_{pu},$$

then

$$\frac{\partial f}{\partial \theta_i} = \xi_{iu}, \qquad i = 1, 2, \ldots, p,$$

and is independent of $\boldsymbol{\theta}$. This leaves the normal equations in the form of linear equations in $\theta_1, \theta_2, \ldots, \theta_p$ as we saw in previous chapters. When the model is nonlinear in the θ's, so will be the normal equations. We now illustrate this with a simple example involving the estimation of a single parameter θ in a nonlinear model.

Example. Suppose we wish to find the normal equation for obtaining the least squares estimate $\hat{\theta}$ of θ for the model $Y = f(\theta, t) + \epsilon$, where $f(\theta, t) = e^{-\theta t}$, and where n pairs of observations $(Y_1, t_1), (Y_2, t_2), \ldots, (Y_n, t_n)$ are available. We find that

$$\frac{\partial f}{\partial \theta} = -te^{-\theta t}.$$

Applying Eq. (24.1.10) leads to the single normal equation

$$\sum_{u=1}^{n} [Y_u - e^{-\hat{\theta} t_u}][-t_u e^{-\hat{\theta} t_u}] = 0$$

or

$$\sum_{u=1}^{n} Y_u t_u e^{-\hat{\theta} t_u} - \sum_{u=1}^{n} t_u e^{-2\hat{\theta} t_u} = 0. \tag{24.1.11}$$

We see that even with one parameter and a comparatively simple nonlinear model, finding $\hat{\theta}$ by solving the (only) normal equation is not easy. When more parameters are involved and the model is more complicated, the solution of the normal equations can be extremely difficult to obtain, and iterative methods must be employed in nearly all cases. To compound the difficulties it may happen that multiple solutions exist, corresponding to multiple stationary values of the function $S(\hat{\boldsymbol{\theta}})$. We now discuss methods that have been used to estimate the parameters in nonlinear systems.

24.2. ESTIMATING THE PARAMETERS OF A NONLINEAR SYSTEM

In some nonlinear problems it is most convenient to write down the normal Eqs. (24.1.10) and develop an iterative technique for solving them. Whether this works satisfactorily or not depends on the form of the equations and the iterative method used. In addition to this approach there are several currently employed methods available for obtaining the parameter estimates by a routine computer calculation. We shall mention three of these: (1) linearization, (2) steepest descent, and (3) Marquardt's compromise.

The linearization (or Taylor series) method uses the results of linear least squares in a succession of stages. Suppose the postulated model is of the form of Eq. (24.1.8). Let $\theta_{10}, \theta_{20}, \ldots, \theta_{p0}$ be initial values for the parameters $\theta_1, \theta_2, \ldots, \theta_p$. These initial values may be intelligent guesses or preliminary estimates based on whatever information is available. (For example, they may be values suggested by the information gained in fitting a similar equation in a different laboratory or suggested as "about right" by the experimenter based on his/her experience and knowledge.) These initial values will, hopefully, be improved upon in the successive iterations to be described below. If we carry out a Taylor series expansion of $f(\boldsymbol{\xi}_u, \boldsymbol{\theta})$ about the point $\boldsymbol{\theta}_0$, where $\boldsymbol{\theta}_0 =$

$(\theta_{10}, \theta_{20}, \ldots, \theta_{p0})'$, and curtail the expansion at the first derivatives, we can say that, approximately, when $\boldsymbol{\theta}$ is close to $\boldsymbol{\theta}_0$,

$$f(\boldsymbol{\xi}_u, \boldsymbol{\theta}) = f(\boldsymbol{\xi}_u, \boldsymbol{\theta}_0) + \sum_{i=1}^{p} \left[\frac{\partial f(\boldsymbol{\xi}_u, \boldsymbol{\theta})}{\partial \theta_i} \right]_{\theta=\theta_0} (\theta_i - \theta_{i0}). \tag{24.2.1}$$

If we set

$$\begin{aligned} f_u^0 &= f(\boldsymbol{\xi}_u, \boldsymbol{\theta}_0), \\ \beta_i^0 &= \theta_i - \theta_{i0}, \\ Z_{iu}^0 &= \left[\frac{\partial f(\boldsymbol{\xi}_u, \boldsymbol{\theta})}{\partial \theta_i} \right]_{\theta=\theta_0}, \end{aligned} \tag{24.2.2}$$

we can see that Eq. (24.1.8) is of the form, approximately,

$$Y_u - f_u^0 = \sum_{i=1}^{p} \beta_i^0 Z_{iu}^0 + \epsilon_u; \tag{24.2.3}$$

in other words it is of the linear form shown in Eq. (24.1.1), to the selected order of approximation. We can now estimate the parameters β_i^0, $i = 1, 2, \ldots, p$, by applying linear least squares theory. If we write

$$\mathbf{Z}_0 = \begin{bmatrix} Z_{11}^0 & Z_{21}^0 & \cdots & Z_{p1}^0 \\ Z_{12}^0 & Z_{22}^0 & \cdots & Z_{p2}^0 \\ \vdots & \vdots & & \vdots \\ Z_{1u}^0 & Z_{2u}^0 & \cdots & Z_{pu}^0 \\ \vdots & \vdots & & \vdots \\ Z_{1n}^0 & Z_{2n}^0 & \cdots & Z_{pn}^0 \end{bmatrix} = \{Z_{iu}^0\}, \qquad n \times p, \tag{24.2.4}$$

$$\mathbf{b}_0 = \begin{bmatrix} b_1^0 \\ b_2^0 \\ \vdots \\ b_p^0 \end{bmatrix} \quad \text{and} \quad \mathbf{y}_0 = \begin{bmatrix} Y_1 - f_1^0 \\ Y_2 - f_2^0 \\ \vdots \\ Y_u - f_u^0 \\ \vdots \\ Y_n - f_n^0 \end{bmatrix} = \mathbf{Y} - \mathbf{f}^0, \tag{24.2.5}$$

say, with an obvious notation, then the estimate of $\boldsymbol{\beta}_0 = (\beta_1^0, \beta_2^0, \ldots, \beta_p^0)'$ is given by

$$\mathbf{b}_0 = (\mathbf{Z}_0'\mathbf{Z}_0)^{-1}\mathbf{Z}_0'(\mathbf{Y} - \mathbf{f}^0). \tag{24.2.6}$$

The vector $\mathbf{b}_0$ will therefore minimize the sum of squares

$$\mathrm{SS}(\boldsymbol{\theta}) \equiv \sum_{u=1}^{n} \left\{ Y_u - f(\boldsymbol{\xi}_u, \boldsymbol{\theta}_0) - \sum_{i=1}^{p} \beta_i^0 Z_{iu}^0 \right\}^2 \tag{24.2.7}$$

with respect to the β_i^0, $i = 1, 2, \ldots, p$, where $\beta_i^0 = \theta_i - \theta_{i0}$. Let us write $b_i^0 = \theta_{i1} - \theta_{i0}$. Then the θ_{i1}, $i = 1, 2, \ldots, p$, can be thought of as the revised best estimates of $\boldsymbol{\theta}$.

Note carefully the difference between the sum of squares $S(\boldsymbol{\theta})$ in Eq. (24.1.9), where the appropriate *nonlinear* model is used, and the sum of squares $\mathrm{SS}(\boldsymbol{\theta})$ in Eq. (24.2.7), where the *approximating linear expansion* of the model is employed.

We can now place the values θ_{i1}, the revised estimates, in the same roles as were played above by the values θ_{i0} and go through exactly the same procedure described above by Eqs. (24.2.1) through (24.2.7), but replacing all the zero subscripts by ones. This will lead to another set of revised estimates θ_{i2}, and so on. In vector form, extending the previous notation in an obvious way, we can write

$$\boldsymbol{\theta}_{j+1} = \boldsymbol{\theta}_j + \mathbf{b}_j \tag{24.2.8}$$

$$\boldsymbol{\theta}_{j+1} = \boldsymbol{\theta}_j + (\mathbf{Z}_j'\mathbf{Z}_j)^{-1}\mathbf{Z}_j'(\mathbf{Y} - \mathbf{f}^j),$$

where

$$\begin{aligned} \mathbf{Z}_j &= \{Z_{iu}^j\}, \\ \mathbf{f}^j &= (f_1^j, f_2^j, \ldots, f_n^j)', \\ \boldsymbol{\theta}_j &= (\theta_{1j}, \theta_{2j}, \ldots, \theta_{pj})'. \end{aligned} \tag{24.2.9}$$

This iterative process is continued until the solution converges, that is, until in successive iterations j, $(j + 1)$,

$$|\{\theta_{i(j+1)} - \theta_{ij}\}/\theta_{ii}| < \delta, \qquad i = 1, 2, \ldots, p,$$

where δ is some prespecified amount (e.g., 0.000001). At each stage of the iterative procedure, $S(\boldsymbol{\theta}_j)$ can be evaluated to see if a reduction in its value has actually been achieved.

The linearization procedure has possible drawbacks for some problems in that:

1. It may converge very slowly; that is, a very large number of iterations may be required before the solution stabilizes even though the sum of squares $S(\boldsymbol{\theta}_j)$ may decrease consistently as j increases. This sort of behavior is not common but can occur.
2. It may oscillate widely, continually reversing direction, and often increasing, as well as decreasing the sum of squares. Nevertheless, the solution may stabilize eventually.
3. It may not converge at all, and even diverge, so that the sum of squares increases iteration after iteration without bound.

To combat these deficiencies, a program written by G. W. Booth and T. I. Peterson (1958), Non-linear estimation, IBM, SHARE Program Pa. No. 687 (WLNLI), under the direction of G. E. P. Box amended the correction vector $\mathbf{b}_j$ in Eq. (24.2.8) by halving it if

$$S(\boldsymbol{\theta}_{j+1}) > S(\boldsymbol{\theta}_j)$$

or doubling it if

$$S(\boldsymbol{\theta}_{j+1}) < S(\boldsymbol{\theta}_j).$$

This halving and/or doubling process is continued until three points between $\boldsymbol{\theta}_j$ and $\boldsymbol{\theta}_{j+1}$ are found, which include between them a local minimum of $S(\boldsymbol{\theta})$. A quadratic interpolation is used to locate the minimum, and the iterative cycle begins again.

Although in theory this method always converges (see Hartley, 1961), in practice difficulties may occur. The linearization method is, in general, a useful one and will successfully solve many nonlinear problems. Where it does not, consideration should be given to reparameterization of the model (see Section 24.4) or to the use of Marquardt's compromise.

A Remark on Derivatives. Many computer programs that use a method needing the values of the derivatives of a function at certain points do not use the functional values of the derivatives at all. Instead they compute ratios such as

$$\{f(\boldsymbol{\xi}_u, \theta_{10}, \theta_{20}, \ldots, \theta_{i0} + h_i, \ldots, \theta_{p0}) - f(\boldsymbol{\xi}_u, \theta_{10}, \theta_{20}, \ldots, \theta_{p0})\}/h_i,$$
$$i = 1, 2, \ldots, p,$$

where h_i is a selected small increment. The ratio given above is an approximation to the expression

$$\left[\frac{\partial f(\boldsymbol{\xi}_u, \boldsymbol{\theta})}{\partial \theta_i}\right]_{\theta=\theta_0}$$

since, if h_i tends to zero, the limit of the ratio is this expression by definition.

A Geometrical Interpretation of Linearization

The sum of squares function $S(\boldsymbol{\theta})$ is a function of the parameter elements of $\boldsymbol{\theta}$ only; the data provide the numerical coefficients in $S(\boldsymbol{\theta})$ and these are fixed for any specific nonlinear estimation problem. In the *parameter space,* that is, the p-dimensional geometrical space of $\theta_1, \theta_2, \ldots, \theta_p$, the function $S(\boldsymbol{\theta})$ can be represented by the contours of a surface. If the model were linear in the θ's, the surface contours would be ellipsoidal and would have a single local (and so a single global) minimum height, $S(\hat{\boldsymbol{\theta}})$, at the location defined by the least squares estimator $\hat{\boldsymbol{\theta}}$. If the model is nonlinear, the contours are not ellipsoidal but tend to be irregular and often "banana-shaped," perhaps with several local minima and perhaps with more than one global minimum, that is, the minimum height may be attained at more than one $\boldsymbol{\theta}$-location. Figure 24.1 provides examples for $p = 2$. Figure 24.1*a* shows the "elliptical bowl" $S(\boldsymbol{\theta})$ contours for a linear model, while Figure 24.1*b* shows the "irregular bowl" $S(\boldsymbol{\theta})$ contours for a nonlinear model.

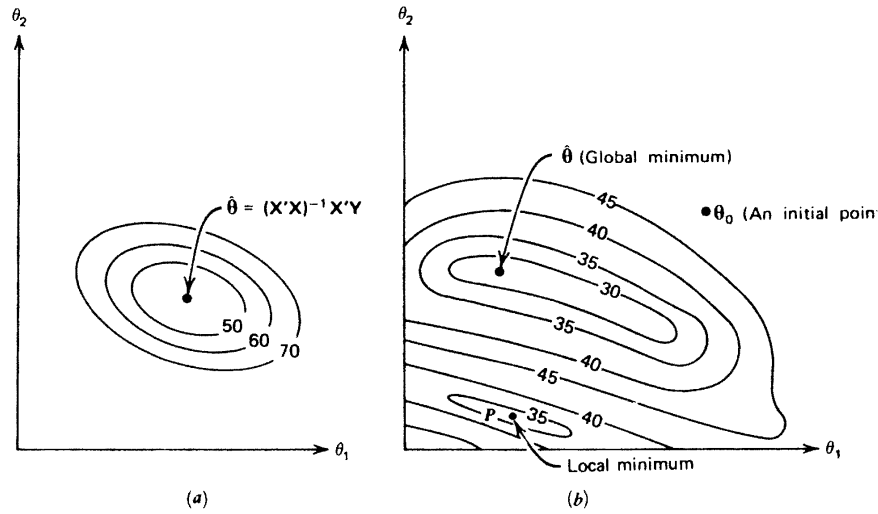

Figure 24.1. (*a*) Elliptical $S(\boldsymbol{\theta})$ contours for a linear model $Y = \theta_1 X_1 + \theta_2 X_2 + \epsilon$; this bowl has a unique minimum point $\hat{\boldsymbol{\theta}}$. (*b*) Irregular $S(\boldsymbol{\theta})$ contours for a nonlinear model, with two local minima. The desired solution is at $\hat{\boldsymbol{\theta}}$ but iteration into point P is possible. Iterative solutions should be obtained starting from several well spread initial points $\boldsymbol{\theta}_0$ as a check.

The precise shape and orientation of the $S(\boldsymbol{\theta})$ contours depend on the model and the data. When the contours surrounding the least squares estimator $\hat{\boldsymbol{\theta}}$ are greatly elongated, and many possible $\boldsymbol{\theta}$-values are "nearly as good" as $\hat{\boldsymbol{\theta}}$ in the sense that their $S(\boldsymbol{\theta})$ "bowl height" values are close to $S(\hat{\boldsymbol{\theta}})$, the problem is said to be ill-conditioned and $\hat{\boldsymbol{\theta}}$ may be difficult to obtain computationally. Ill-conditioning could indicate a model that is overparameterized, that is, one that has more parameters than are needed, or inadequate data that will not allow us to estimate the parameters postulated. Because these are two sides of the same coin, the choice of whether one or the other is the culprit depends on one's prior knowledge about the practical problem and one's point of view. For example, consider $f(t; \theta_1, \theta_2)$ in Eq. (24.1.3), which represents a curve that begins (at $t = 0$) and ends (at $t = \infty$) at height zero, and rises to a peak somewhere in between. The slope at $t = 0$ is θ_1, and the peak is at

$$t_{\text{peak}} = \ln(\theta_1/\theta_2)/(\theta_1 - \theta_2).$$

It follows that, if our data cover just the early part of the curve (see Figure 24.2*a*) we shall be able to estimate θ_1 well, but not θ_2. For the latter we must obtain information on where the curve peaks as in Figure 24.2*b*. A one-parameter model $Y = \theta t + \epsilon$ would be adequate for the data of Figure 24.2*a*; these data are inadequate for estimating the two-parameter model, Eq. (24.1.3).

The linearization method converts the problem of finding the minimum height of $S(\boldsymbol{\theta})$ for a nonlinear model starting from an initial point $\boldsymbol{\theta}_0$, into a series of linear model problems. The initial linearization Eq. (24.2.1) of $f(\boldsymbol{\xi}, \boldsymbol{\theta})$ about $\boldsymbol{\theta}_0$ replaces the irregular $S(\boldsymbol{\theta})$ bowl by an elliptical bowl $SS(\boldsymbol{\theta})$ that "looks the right shape," that is, has the same first derivatives of the corresponding model function right at $\boldsymbol{\theta}_0$. As we shall see in the example of Section 24.3, it may approximate the actual $S(\boldsymbol{\theta})$ contours badly or well, depending on the actual circumstances, namely, the model assumed, the data available, and the relative positions of $\boldsymbol{\theta}_0$ and $\hat{\boldsymbol{\theta}}$ in the $\boldsymbol{\theta}$-space. In any event we solve the "linearized at $\boldsymbol{\theta}_0$" problem by moving to the bottom point of the linearized bowl at $\boldsymbol{\theta}_0$ (a relatively easy linear-least-squares calculation) to reach $\boldsymbol{\theta}_1$ as shown in Figure 24.3. Then we repeat the whole linearization process at $\boldsymbol{\theta}_1$. Our hope is that the successive iterations will converge to $\hat{\boldsymbol{\theta}}$, as indicated in Figure 24.4, rather than diverge. Typically, linearization does well when the starting point of the iteration is close to $\hat{\boldsymbol{\theta}}$, because the actual contours are then usually well approximated by the linearized ones.

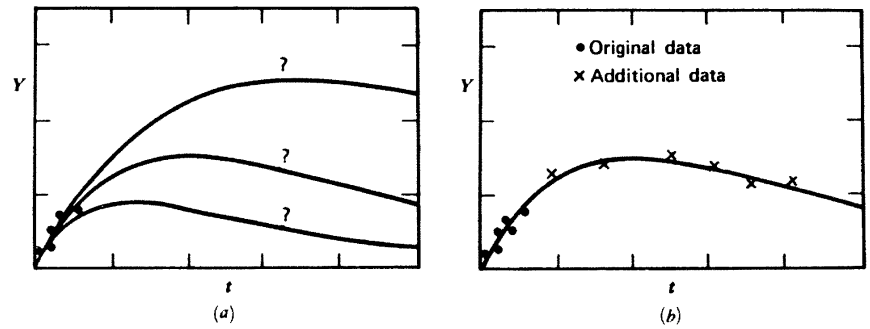

Figure 24.2. (*a*) These data would allow us to estimate the initial slope θ_1 but not where the curve peaked, which involves θ_2 as well. The $S(\boldsymbol{\theta})$ surface would be ill-conditioned if Eq. (24.1.3) were used. (*b*) Additional data shown would enable us to estimate both θ_1 *and* θ_2 well in Eq. (24.1.3) and the $S(\boldsymbol{\theta})$ surface would now be comparatively well-conditioned.

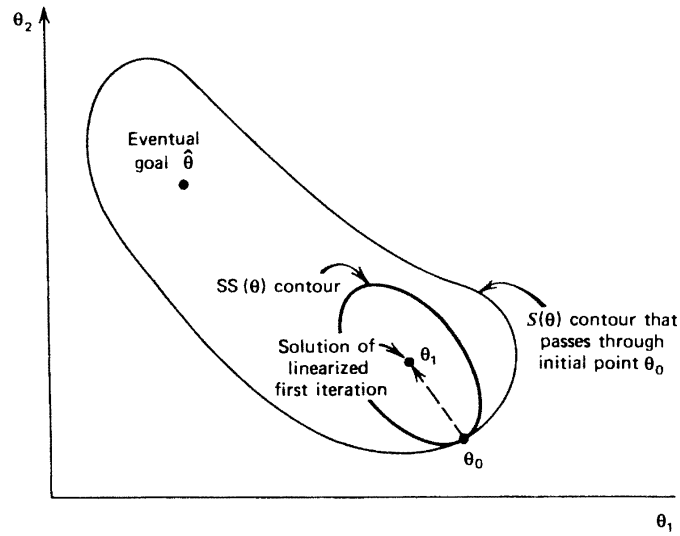

Figure 24.3. A first iteration in the linearization process. The ellipse of the SS($\boldsymbol{\theta}$) contour "fits closely" to the $S(\boldsymbol{\theta})$ contour at $\boldsymbol{\theta}_0$, in the sense described in the text. The linearized problem provides the solution $\boldsymbol{\theta}_1$, and the procedure is then repeated from there.

More detail on the geometry of linear and nonlinear least squares is given in Sections 24.5 and 24.6.

Steepest Descent

The steepest descent method involves concentration on the sum of squares function, $S(\boldsymbol{\theta})$ as defined by Eq. (24.1.9), and use of an iterative process to find the minimum

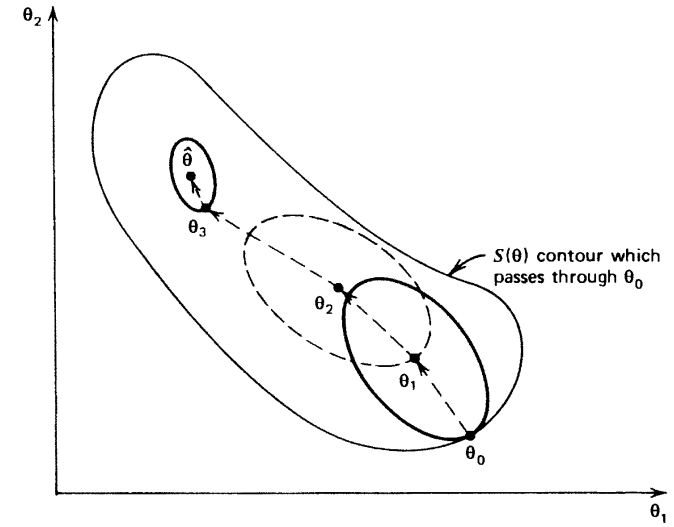

Figure 24.4. Successive iterations of a linearization procedure shown converging to the point $\hat{\boldsymbol{\theta}}$, where minimum $S(\boldsymbol{\theta})$ is attained. Convergence is guaranteed by theory but, in practice, the process may diverge.

of this function. The basic idea is to move, from an initial point $\boldsymbol{\theta}_0$, along the vector with components

$$-\frac{\partial S(\boldsymbol{\theta})}{\partial \theta_1}, -\frac{\partial S(\boldsymbol{\theta})}{\partial \theta_2}, \ldots, -\frac{\partial S(\boldsymbol{\theta})}{\partial \theta_p},$$

whose values change continuously as the path is followed. One way of achieving this in practice, without evaluating functional derivatives, is to estimate the vector slope components at various places on the surface $S(\boldsymbol{\theta})$ by fitting planar approximating functions. This is a technique of great value in experimental work for finding stationary values of response surfaces. A full description of the method is given in Box and Draper (1987) and we shall discuss it only briefly here.

The procedure is as follows. Starting in one particular region of the $\boldsymbol{\theta}$-space (or the *parameter space* as we shall call it) several *runs* are made, by selecting n (say) combinations of levels of $\theta_1, \theta_2, \ldots, \theta_p$ and evaluating $S(\boldsymbol{\theta})$ at those combinations of levels. The runs are usually chosen in the pattern of a two-level factorial design. Using the evaluated $S(\boldsymbol{\theta})$ values as observations of a dependent variable and the combinations of levels of $\theta_1, \theta_2, \ldots, \theta_p$ as the observations of corresponding predictor variables, we fit the model

$$\text{"Observed } S(\boldsymbol{\theta})\text{"} = \beta_0 + \sum_{i=1}^{p} \beta_i(\theta_i - \bar{\theta}_i)/s_i + \epsilon$$

by standard least squares. Here $\bar{\theta}_i$ denotes the mean of the levels θ_{iu}, $u = 1, 2, \ldots, n$, of θ_i used in the runs, and s_i is a scaling factor chosen so that $\Sigma_{u=1}^{n} (\theta_{iu} - \bar{\theta}_i)^2/s_i^2 =$ constant. This implies that we believe the true surface defined by $S(\boldsymbol{\theta})$ can be approximately represented by a plane in the region of the parameter space in which we made our runs. The estimated coefficients

$$b_1, b_2, \ldots, b_p$$

indicate the direction of steepest ascent so the negatives of these, namely,

$$-b_1, -b_2, \ldots, -b_p$$

indicate the direction of steepest descent. This means that as long as the linear approximation is realistic the maximum decrease in $S(\boldsymbol{\theta})$ will be obtained by moving along the line which contains points such that

$$(\theta_i - \bar{\theta}_i)/s_i \propto -b_i.$$

Denoting the proportionality factor by λ, the path of steepest descent contains points $(\theta_1, \theta_2, \ldots, \theta_p)$ such that

$$\frac{(\theta_i - \bar{\theta}_i)}{s_i} = -\lambda b_i,$$

where $\lambda > 0$, or

$$\theta_i = \bar{\theta}_i - \lambda b_i s_i.$$

By giving λ selected values the path of steepest descent can be followed. A number of values of λ are selected and the path of steepest descent is followed as long as $S(\boldsymbol{\theta})$ decreases. When it does not, another experimental design is set down and the process is continued until it converges to the value $\hat{\boldsymbol{\theta}}$ that minimizes $S(\boldsymbol{\theta})$.

While, theoretically, the steepest descent method will converge, it may do so in practice with agonizing slowness after some rapid initial progress. Slow convergence is particularly likely when the $S(\boldsymbol{\theta})$ contours are attenuated and banana-shaped (as they often are in practice), and it happens when the path of steepest descent zigzags slowly up a narrow ridge, each iteration bringing only a slight reduction in $S(\boldsymbol{\theta})$. (This is less of a problem in laboratory-type investigations where human intervention can be permitted at each stage of calculation since then the experimental design can be revised, the scales of the independent variables can be changed, and so on.) This difficulty has led to modifications of the basic steepest descent procedure when used for nonlinear fitting. For some references see Spang (1962). (One possible modification is to use a second-order approximating function rather than a first-order or planar approximation. While this provides better graduation of the true surface, it also requires additional computation in the iterative procedures.)

A further disadvantage of the steepest descent method is that it is not scale invariant. The indicated direction of movement changes if the scales s_i of the variables are changed, unless all are changed by the same factor. The steepest descent method is, on the whole, slightly less favored than the linearization method but will work satisfactorily for many nonlinear problems, especially if modifications are made to the basic technique.

On the whole, steepest descent works well when the current position in the $\boldsymbol{\theta}$-space is far from the desired $\hat{\boldsymbol{\theta}}$, which is usually so in the early iterations. As $\hat{\boldsymbol{\theta}}$ is approached, the "zigzagging" behavior of steepest descent previously described is likely, and linearization tends to work better. The Marquardt procedure, based on work by Levenberg (1944), takes account of these facts.

Marquardt's Compromise

A method developed by Marquardt (1963) enlarged considerably the number of practical problems that can be tackled by nonlinear estimation. Marquardt's method represents a compromise between the linearization (or Taylor series) method and the steepest descent method and appears to combine the best features of both while avoiding their most serious limitations. It is good in that it almost always converges and does not "slow down" as the steepest descent method often does. However, as we again emphasize, the other methods will work perfectly well on many practical problems that do not violate the limitations of the methods. (In general, we must keep in mind that, given a particular method, a problem can usually be constructed to defeat it. Alternatively, given a particular problem and a suggested method, ad hoc modifications can often provide quicker convergence than an alternative method. The Marquardt method is one that appears to work well in many circumstances and thus is a sensible practical choice. For the reasons stated above, no method can be called "best" for all nonlinear problems.)

The idea of Marquardt's method can be explained briefly as follows. Suppose we start from a certain point in the parameter space, $\boldsymbol{\theta}$. If the method of steepest descent is applied, a certain vector direction, $\boldsymbol{\delta}_g$, where g stands for gradient, is obtained for movement away from the initial point. Because of attenuation in the $S(\boldsymbol{\theta})$ contours this may be the best *local* direction in which to move to attain smaller values of $S(\boldsymbol{\theta})$ but may not be the best *overall* direction. However, the best direction must be within 90° of $\boldsymbol{\delta}_g$ or else $S(\boldsymbol{\theta})$ will get larger locally. The linearization (or Taylor series) method leads to another correction vector $\boldsymbol{\delta}$ given by a formula like Eq. (24.2.6). Marquardt found that for a number of practical problems he studied, the angle, ϕ say, between

$\boldsymbol{\delta}_g$ and $\boldsymbol{\delta}$ fell in the range $80° < \phi < 90°$. In other words, the two directions were almost at right angles! The Marquardt algorithm provides a method for interpolating between the vectors $\boldsymbol{\delta}_g$ and $\boldsymbol{\delta}$ and for obtaining a suitable step size as well.

We shall not go into the detail of the method here. The basic algorithm is given in the quoted reference. See also Bates and Watts (1988) and Seber and Wild (1989).

Confidence Contours

Some idea of the nonlinearity in the model under study can be obtained, after the estimation of $\boldsymbol{\theta}$, by evaluating the ellipsoidal confidence region obtained on the assumption that the linearized form of the model is valid around $\hat{\boldsymbol{\theta}}$, the final estimate of $\boldsymbol{\theta}$. This is given by the formula

$$(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})'\hat{\mathbf{Z}}'\mathbf{Z}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}) \leq ps^2F(p, n - p, 1 - \alpha),$$

where $\hat{\mathbf{Z}}$ denotes a matrix of the form shown in Eq. (24.2.4) but with $\hat{\boldsymbol{\theta}}$ substituted into the elements in place of $\boldsymbol{\theta}_0$ everywhere, and where

$$s^2 = S(\hat{\boldsymbol{\theta}})/(n - p).$$

Note that when the difference between successive values $\boldsymbol{\theta}_{j+1}$ and $\boldsymbol{\theta}_j$ is sufficiently small so that the linearization procedure terminates with $\boldsymbol{\theta}_{j+1} = \hat{\boldsymbol{\theta}}$ $(= \boldsymbol{\theta}_j$ for practical purposes), then $S(\hat{\boldsymbol{\theta}})$ is a minimum value of $S(\boldsymbol{\theta})$ in Eq. (24.1.9) to the accuracy imposed by the termination procedure selected. This can be seen by examining Eq. (24.2.7) with $\hat{\boldsymbol{\theta}}$, β_i^{j+1}, and Z_{iu}^{j+1} replacing $\boldsymbol{\theta}_0$, β_i^0, and Z_{iu}^0, respectively, and remembering that, to the order of accuracy imposed by the termination procedure, $\mathbf{b}_{j+1} = \mathbf{0}$. The ellipsoid above will *not* be a true confidence region when the model is nonlinear. We can, however, determine the end points on the major axes of this ellipsoid by canonical reduction (see, e.g., Box and Draper, 1987). The *actual* values of $S(\boldsymbol{\theta})$ can be evaluated at these points and compared with each other. Under linear theory the values would all be the same.

An exact confidence contour is defined by taking $S(\boldsymbol{\theta})$ = constant, but since we do not know the correct distribution properties in the general nonlinear case, we are unable to obtain a specified probability level. However, we can, for example, choose the contour such that

$$S(\boldsymbol{\theta}) = S(\hat{\boldsymbol{\theta}})\left\{1 + \frac{p}{n - p}F(p, n - p, 1 - \alpha)\right\},$$

which, if the model is linear, provides an *exact*, ellipsoidal $100(1 - \alpha)\%$ boundary, and label it as an approximate $100(1 - \alpha)\%$ confidence contour in the nonlinear case. Note that the contour so determined *will be a proper correct confidence contour in this case* (and will not be elliptical in general), *and it is only the probability level that is approximate.* When only two parameters are involved the confidence contour can be drawn. For more parameters, sectional drawings can be constructed if desired.

In general, when a linearized form of a nonlinear model is used, all the usual formulas and analyses of linear regression theory can be applied. Any results obtained, however, are valid only to the extent that the linearized form provides a good approximation to the true model.

Grids and Plots

Two obvious ways of examining the sum of squares surface $S(\boldsymbol{\theta})$ are often overlooked; they can be particularly useful when an iterative procedure, beginning from chosen values, does not satisfactorily converge.

The first of these is to select a grid of points, that is, a factorial design, in the space of the parameters $(\theta_1, \theta_2, \ldots, \theta_p)$ and to evaluate (usually on a computer) the sum of squares function at every point of the grid. These values will provide some idea of the form of the sum of squares surface and may reveal, for example, that multiple minima are possible. In any case, the grid point at which the smallest sum of squares is found can be used as the starting point of an iterative parameter estimation procedure, or a reduced grid can be examined in the best neighborhood, to obtain a better starting point. The simplest type of grid available is that in which *two* levels of every parameter are selected. In this case, the grid points are those of a 2^p factorial design, and it is possible to use standard methods to evaluate the factorial effects and interactions and so provide information on the effects of changes in the parameters on the sum of squares function $S(\boldsymbol{\theta})$.

The second possibility is to draw sum of squares contours in any particular region of the parameter space in which difficulty in convergence occurs or in which additional information would be helpful. This is usually straightforward when only one or two parameters are involved. When there are more than two parameters, two-dimensional slices of the contours can be obtained for selected values of all but two of the parameters, and a composite picture can be built up.

The Importance of Good Starting Values

All iterative procedures require initial values $\theta_{10}, \theta_{20}, \ldots, \theta_{p0}$, of the parameters $\theta_1, \theta_2, \ldots, \theta_p$, to be selected. All available prior information should be used to make these starting values as reliable as they possibly can be. Good starting values will often allow an iterative technique to converge to a solution much faster than would otherwise be possible. Also, if multiple minima exist or if there are several local minima in addition to an absolute minimum, poor starting values may result in convergence to an unwanted stationary point of the sum of squares surface. This unwanted point may have parameter values that are physically impossible or that do not provide the true minimum value of $S(\boldsymbol{\theta})$. As suggested above, a preliminary evaluation of $S(\boldsymbol{\theta})$ at a number of grid points in the parameter space is often useful.

Getting Initial Estimates $\boldsymbol{\theta}_0$

There is no standard "crank the handle" mechanism for getting initial estimates $\boldsymbol{\theta}_0$ for every nonlinear estimation problem. Methods that have worked in various problems are the following:

1. If there are p parameters, substitute for p sets of observations $(Y_u, \boldsymbol{\xi}_u)$ into the postulated model *ignoring the error.* Solve the resulting p equations for the parameters (if possible). Widely separated $\boldsymbol{\xi}_u$ often work best.

2. In approach (1), or sometimes as an alternative to it, consider the behavior of the response function as the ξ_i go to zero or infinity, and substitute in for observations that most nearly represent those conditions in the scale and context of the problem. Solve (if possible) the resulting equations.

3. Check the form of the model to see if (were it not for the additive error) the model could be transformed approximately. For example, if the model is $Y = \theta_1 e^{-\theta_2 t} + \epsilon$, a plot of ln Y versus t will usually give good initial estimates of ln θ_1 and $-\theta_2$ obtained from the intercept and slope of the ln Y versus t plot. (This is based on

the idea that if the model had been $Y = \theta_1 e^{-\theta_2 t}\epsilon$ instead, the transformation $\ln Y = \ln \theta_1 - \theta_2 t + \ln \epsilon$ would work.)

4. A more complicated example of (3) is given by the model $\ln W = -\theta_1^{-1} \ln(\theta_2 + \theta_3 X^{\theta_4}) + \epsilon$, a model useful in growth studies. (for source details, see Mead, 1970.) A plot of W^{-1} versus X would be a straight line with intercept θ_2 and slope θ_3, *if* $\theta_1 = \theta_4 = 1$. If this plot is curved, then trial and error can be used to search for values of θ_1 and θ_4 that make the plot of $W^{-\theta_1}$ versus X^{θ_4} into a "good" straight line. Once this has been achieved to whatever extent possible, the corresponding θ-values are the initial estimates. Note that, in models like this, poor initial estimates may cause the argument $\theta_2 + \theta_3 X^{\theta_4}$ to go negative, creating computing problems; good initial estimates will often prevent the occurrence of such problems.

5. If all else fails, grids and plots can be used—see above.

Note: When small initial values are chosen initially, or are expected in subsequent iterations, for some parameters, care must be taken to see that the intervals h_i used to evaluate the corresponding numerical partial derivatives are taken suitably small. Some routines fail if this is not done appropriately.

24.3. AN EXAMPLE

The example that follows is taken from an investigation performed at Procter & Gamble and reported by Smith and Dubey (1964). We shall use this example to illustrate how a solution can be obtained for a nonlinear estimation problem by solving the normal equations directly, or alternatively by the linearization method. We shall not provide an example of the use of steepest descent (but see, e.g., Box and Coutie, 1956), nor an example of Marquardt's compromise procedure. The investigation involved a product A, which must have a fraction of 0.50 of Available Chlorine at the time of manufacture. The fraction of Available Chlorine in the product decreases with time; this is known. In the 8 weeks before the product reaches the consumer a decline to a level 0.49 occurs but since many uncontrolled factors then arise (such as warehousing environments, handling facilities), theoretical calculations are not reliable for making extended predictions of the Available Chlorine fraction present at later times. To assist management in decisions—such as (1) When should warehouse material be scrapped? and (2) When should store stocks be replaced?—cartons of the product were analyzed over a period to provide the data of Table 24.2. (Note that the product is made only every other week and code-dated only by the week of the year. The predicted values shown in the table are obtained from the fitted equation to be found in what follows.) It was postulated that a nonlinear model of the form

$$Y = \alpha + (0.49 - \alpha)e^{-\beta(X-8)} + \epsilon \tag{24.3.1}$$

would suitably account for the variation observed in the data, for $X \geq 8$. This model provides a true level, without error, of $\eta = 0.49$ when $X = 8$, and it exhibits the proper sort of decay. An additional point of information, agreed upon by knowledgeable chemists, was that an equilibrium, asymptotic level of Available Chlorine somewhere above 0.30 should be expected. The problem is to estimate the parameters α and β of the nonlinear model given in Eq. (24.3.1) using the data given in the table. The residual sum of squares for this model can be written as

$$S(\alpha, \beta) = \sum_{u=1}^{n} [Y_u - \alpha - (0.49 - \alpha)e^{-\beta(X_u-8)}]^2, \tag{24.3.2}$$

TABLE 24.2. Percent of Available Chlorine in a Unit of Product

Length of Time Since Produced (weeks) X	Available Chlorine Y	Average Available Chlorine $\bar{Y}$	Predicted Y, Using the Model $\hat{Y}$
8	0.49, 0.49	0.490	0.490
10	0.48, 0.47, 0.48, 0.47	0.475	0.472
12	0.46, 0.46, 0.45, 0.43	0.450	0.457
14	0.45, 0.43, 0.43	0.437	0.445
16	0.44, 0.43, 0.43	0.433	0.435
18	0.46, 0.45	0.455	0.427
20	0.42, 0.42, 0.43	0.423	0.420
22	0.41, 0.41, 0.40	0.407	0.415
24	0.42, 0.40, 0.40	0.407	0.410
26	0.41, 0.40, 0.41	0.407	0.407
28	0.41, 0.40	0.405	0.404
30	0.40, 0.40, 0.38	0.393	0.401
32	0.41, 0.40	0.405	0.399
34	0.40	0.400	0.397
36	0.41, 0.38	0.395	0.396
38	0.40, 0.40	0.400	0.395
40	0.39	0.390	0.394
42	0.39	0.390	0.393

where (X_u, Y_u), $u = 1, 2, 3, \ldots, 44$, are the corresponding pairs of observations from the table (e.g., $X_1 = 8$, $Y_1 = 0.49, \ldots, X_{44} = 42$, $Y_{44} = 0.39$).

A Solution Through the Normal Equations

Differentiating Eq. (24.3.2) first with respect to α, and then with respect to β, and setting the results equal to zero provides two normal equations. After removal of a factor of 2 from the first equation and a factor of $2(0.49 - \alpha)$ from the second equation and some rearrangement, the equations reduce to

$$\alpha = \frac{\Sigma Y_u - \Sigma Y_u e^{-\beta t_u} - 0.49 \Sigma e^{-\beta t_u} + 0.49 \Sigma e^{-2\beta t_u}}{n - 2\Sigma e^{-\beta t_u} + \Sigma e^{-2\beta t_u}} \tag{24.3.3}$$

and

$$\alpha = \frac{0.49 \Sigma t_u e^{-2\beta t_u} - \Sigma Y_u t_u e^{-\beta t_u}}{\Sigma t_u e^{-2\beta t_u} - \Sigma t_u e^{-\beta t_u}}, \tag{24.3.4}$$

where all summations are from $u = 1$ to $u = 44$, and $t_u = X_u - 8$. We see that these normal equations have a particular simplification in that the parameter α can be eliminated by subtracting one equation from the other. If this is done, a single nonlinear equation of the form $f(\beta) = 0$ in β results. This can be solved by applying the Newton–Raphson technique, first guessing a value for β, call it β_0, and then "correcting" it by h_0 obtained as follows. If the root of $f(\beta) = 0$ is at $(\beta_0 + h_0)$, then

$$0 = f(\beta_0 + h_0) = f(\beta_0) + h_0 \left[\frac{df(\beta)}{d\beta} \right]_{\beta=\beta_0} \tag{24.3.5}$$

approximately, or

$$h_0 = -f(\beta_0) \Big/ \left[\frac{df(\beta)}{d\beta}\right]_{\beta=\beta_0} \tag{24.3.6}$$

approximately. We can now use $\beta_1 = \beta_0 + h_0$ instead of β_0 and repeat the correction procedure to find h_1 and so $\beta_2 = \beta_1 + h_1$. This process can be continued until it converges to a value $\hat{\beta}$, which is then the least squares estimate of β. The value of $\hat{\alpha}$, the least squares estimate of α, can be obtained from Eqs. (24.3.3) and (24.3.4) by substituting $\hat{\beta}$ in the right-hand sides. As a check, the same value should be obtained from both equations.

We can guess β_0 initially by noting, for example, that when $X_{44} = 42$, $Y_{44} = 0.39$. If Y_{44} contained no error then we should have

$$0.39 = \alpha + (0.49 - \alpha)e^{-34\beta_0},$$

whereas if we assume that Y tends to 0.30 as X tends to infinity (on the basis of the prior information given by the chemists) then we can make an initial guess of $\alpha_0 = 0.30$ for α, from which it follows that

$$0.39 = 0.30 + (0.49 - 0.30)e^{-34\beta_0}$$

or

$$e^{-34\beta_0} = \frac{0.09}{0.19}$$

so that

$$\beta_0 = \frac{-[\ln(0.09/0.19)]}{34} = 0.02$$

approximately. (Note that we must have $\beta > 0$ or else a decay cannot be represented by the function.)

If we denote Eqs. (24.3.3) and (24.3.4) by

$$\begin{aligned} \alpha &= f_1(\beta), \\ \alpha &= f_2(\beta), \end{aligned} \tag{24.3.7}$$

respectively, then

$$f(\beta) \equiv f_1(\beta) - f_2(\beta) = 0 \tag{24.3.8}$$

and

$$\frac{\partial f(\beta)}{\partial \beta} \equiv \frac{\partial f_1(\beta)}{\partial \beta} - \frac{\partial f_2(\beta)}{\partial \beta}. \tag{24.3.9}$$

Rather than write down the rather lengthy expressions that result from the differentiation of $f_1(\beta)$ and $f_2(\beta)$ we shall adopt a simpler method of finding $\hat{\alpha}$, $\hat{\beta}$.

An alternative procedure for estimating α and β in this case is to plot the functions (24.3.7) over a reasonable range of β and note where the two curves intersect. This provides both $\hat{\alpha}$ and $\hat{\beta}$ immediately since the point of intersection is at $(\hat{\beta}, \hat{\alpha})$. Some

TABLE 24.3. Points on the Curves $f_i(\beta)$

β	$f_1(\beta)$	$f_2(\beta)$
0.06	0.3656	0.3627
0.07	0.3743	0.3720
0.08	0.3808	0.3791
0.09	0.3857	0.3847
0.10	0.3896	0.3894
0.11	0.3927	0.3935
0.12	0.3953	0.3970
0.13	0.3975	0.4002
0.14	0.3993	0.4031
0.15	0.4009	0.4057
0.16	0.4023	0.4082

values of $f_1(\beta)$ and $f_2(\beta)$ for a range of values of β are shown in Table 24.3 and the resulting plot is shown in Figure 24.5. The estimates can be read off squared paper to sufficient accuracy as $\hat{\alpha} = 0.30$, $\hat{\beta} = 0.10$. We can see from the figure that the two curves plotted are quite close together for a comparatively large range of β and for a somewhat smaller range of α. This indicates that β is somewhat less well determined than α. For example, $|f_1(\beta) - f_2(\beta)| < 0.0025$ is achieved by a range of values of β between about 0.07 and 0.12 and a range of values of α between about 0.37 and 0.40. Many pairs of values of (β, α) such as, for example, (0.09, 0.385), (0.11, 0.393) bring the two curves of the figure almost together, and thus do not appear unreasonable estimates for (β, α) in the light of the data even though they do not actually minimize $S(\alpha, \beta)$. We shall see that these comments are substantiated by the confidence regions for the true (β, α), which can be constructed for this problem (see Figure 24.8). The fitted equation now takes the form

$$\hat{Y} = 0.39 + 0.10e^{-0.10(X-8)}. \tag{24.3.10}$$

The observed values of X can be inserted in this equation to give the fitted values

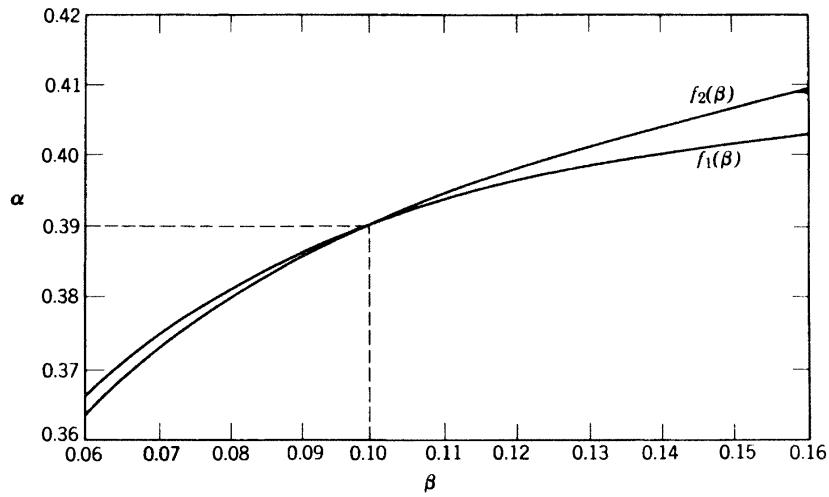

Figure 24.5. Finding $(\hat{\beta}, \hat{\alpha})$ as the intersection of $f_1(\beta)$ and $f_2(\beta)$.

shown in Table 24.2. The fitted curve and the observations are shown in Figure 24.6. The usual analysis of residuals could now be carried out. (The large residuals at $X = 18$ strike the eye immediately. According to the authors no assignable cause could be found for these.)

A Solution Through the Linearization Technique

To linearize the model into the form of Eq. (24.2.1) we need to evaluate the first derivatives of

$$\begin{aligned} f(\boldsymbol{\xi}_u, \boldsymbol{\theta}) &= f(\mathbf{X}_u; \alpha, \beta) \\ &= \alpha + (0.49 - \alpha)e^{-\beta(X_u - 8)}, \end{aligned} \tag{24.3.11}$$

namely,

$$\begin{aligned} \frac{\partial f}{\partial \alpha} &= 1 - e^{-\beta(X_u - 8)}, \\ \frac{\partial f}{\partial \beta} &= -(0.49 - \alpha)(X_u - 8)e^{-\beta(X_u - 8)}. \end{aligned} \tag{24.3.12}$$

Thus if $\alpha = \alpha_j$, $\beta = \beta_j$ are the values inserted at the jth stage, as described in Section 24.2, we have, in the notation implied in that section, a model of form (at the jth stage)

$$\begin{aligned} Y_u - f_u^j = &[1 - e^{-\beta_j(X_u - 8)}](\alpha - \alpha_j) \\ &+ [-(0.49 - \alpha_j)(X_u - 8)e^{-\beta_j(X_u - 8)}](\beta - \beta_j) + \epsilon, \end{aligned}$$

or in matrix form

$$\mathbf{Y} - \mathbf{f}^j = \mathbf{Z}_j \begin{bmatrix} \alpha - \alpha_j \\ \beta - \beta_j \end{bmatrix} + \boldsymbol{\epsilon},$$

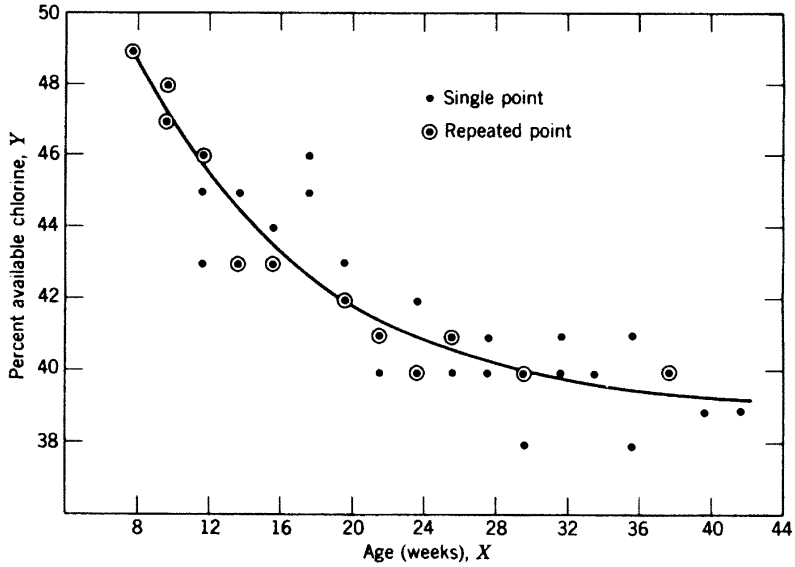

Figure 24.6. The fitted curve and the observations.

where

$$f_u^j = \alpha_j + (0.49 - \alpha_j)e^{-\beta_j(X_u - 8)} \tag{24.3.13}$$

$$\mathbf{Z}_j = \begin{bmatrix} 1 - e^{-\beta_j(X_1-8)} & -(0.49-\alpha_j)(X_1-8)e^{-\beta_j(X_1-8)} \\ \vdots & \vdots \\ 1 - e^{-\beta_j(X_u-8)} & -(0.49-\alpha_j)(X_u-8)e^{-\beta_j(X_u-8)} \\ \vdots & \vdots \\ 1 - e^{-\beta_j(X_n-8)} & -(0.49-\alpha_j)(X_n-8)e^{-\beta_j(X_n-8)} \end{bmatrix}, \tag{24.3.14}$$

and the vector of quantities to be estimated is

$$\begin{bmatrix} \alpha - \alpha_j \\ \beta - \beta_j \end{bmatrix} \tag{24.3.15}$$

with estimate given by

$$\begin{bmatrix} \alpha_{j+1} - \alpha_j \\ \beta_{j+1} - \beta_j \end{bmatrix} = (\mathbf{Z}_j'\mathbf{Z}_j)^{-1}\mathbf{Z}_j' \begin{bmatrix} Y_1 - f_1^j \\ Y_2 - f_2^j \\ \vdots \\ Y_n - f_n^j \end{bmatrix}. \tag{24.3.16}$$

If we begin the iterations with initial guesses $\alpha_0 = 0.30$ and $\beta_0 = 0.02$ as before, and apply Eq. (24.3.16) iteratively, we obtain estimates as follows:

Iteration	α_j	β_j	$S(\alpha_j, \beta_j)$
0	0.30	0.02	0.0263
1	0.8416	0.1007	4.4881
2	0.3901	0.1004	0.0050
3	0.3901	0.1016	0.0050
4	0.3901	0.1016	0.0050

Note: These figures were rounded from the end results of computer calculations, which carried more significant figures. Numerical differences might occur if a parallel calculation were made on a pocket calculator.

This process converges to the same least squares estimates as before, namely, $\hat{\alpha} = 0.39$ and $\hat{\beta} = 0.10$ to give the fitted model, Eq. (24.3.10). Note that this happens in spite of the rather alarming fact that, after the first stage, $S(\alpha_1, \beta_1) = 4.4881$, which is about 170 times the initial $S(\alpha_0, \beta_0) = 0.0263$. The reduction in the next iteration is dramatic and practically final, the subsequent reduction in $S(\alpha, \beta)$ being in the sixth place of decimals, which is not shown. In some nonlinear problems no correction, dramatic or otherwise, occurs and the process diverges, providing larger and larger values for $S(\boldsymbol{\theta})$. (For a possible reason for this sort of behavior, see Section 24.6.)

Figure 24.7*a* shows the nonlinear sum of squares contours $S(\alpha, \beta)$ in the region $0 \le \beta \le 0.20$, $0.28 \le \alpha \le 0.90$ together with the progress from the initial point (β_0, α_0) to (β_2, α_2). The reason for this path is shown in Figures 24.7*b* and 24.7*c*. In Figure 24.7*b* the $\mathrm{SS}(\boldsymbol{\theta})$ contours are relatively ill-conditioned and lead to a minimum $\mathrm{SS}(\alpha, \beta)$ value at a point (β_1, α_1) well away from the actual minimum of $S(\alpha, \beta)$. In the next iteration the linearized sum of squares contours are relatively well-conditioned (Figure 24.7*c*) and also their center happens to be close to the minimum point of the

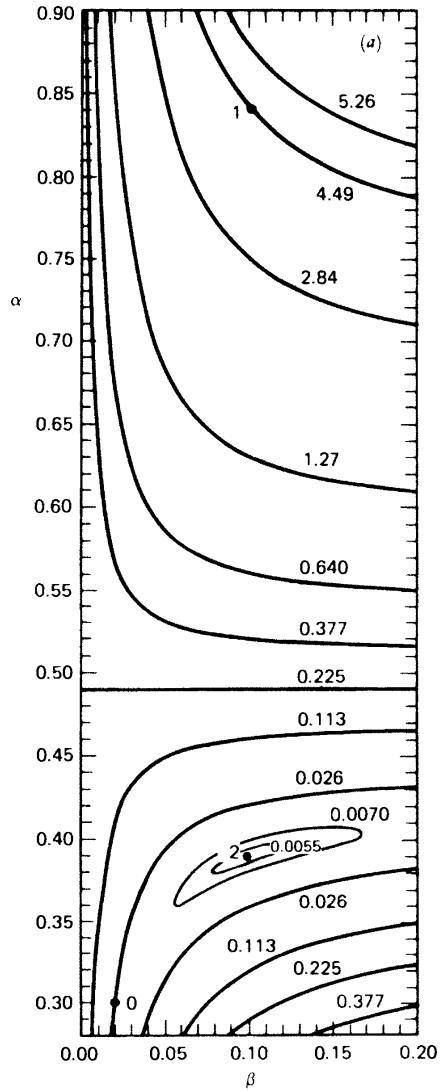

Figure 24.7. (*a*) Nonlinear sum of squares contours $S(\alpha, \beta)$ for the example. The points marked 0, 1, 2 are the (β_i, α_i) for the initial point and the first and second iterations.

actual sum of squares contours, as we have seen. Note that, in both Figures 24.7*b* and 24.7*c*, the direction of steepest descent, which would be perpendicular to the $S(\alpha, \beta)$ contours at the starting point, would take us off in a different direction from that determined by linearization.

Further Analysis

The usual tests appropriate in the linear model case are, in general, *not* appropriate when the model is nonlinear. As a practical procedure we can compare the unexplained variation with an estimate of $V(Y_u) = \sigma^2$ but cannot use the F-statistic to obtain conclusions at any stated level. The unexplained variation is $S(\hat{\alpha}, \hat{\beta}) = 0.0050$. In the absence of exact results for the nonlinear case, we can regard this

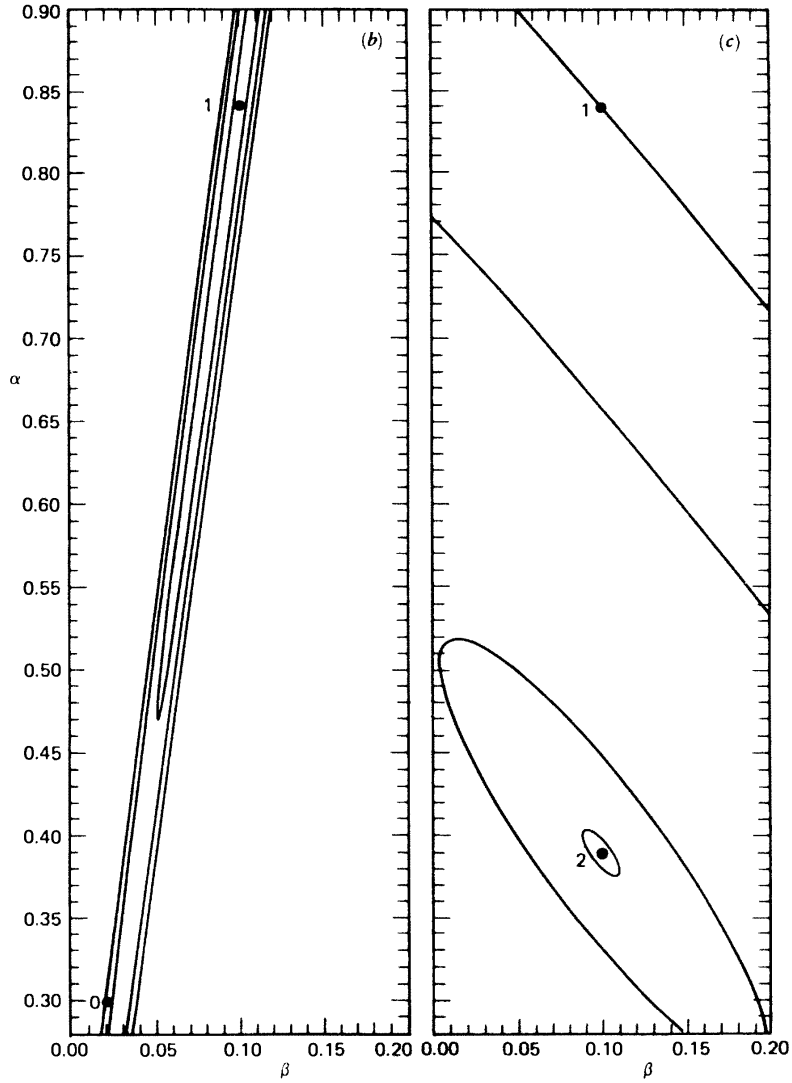

Figure 24.7. (*Continued*) (*b*) Linearized sum of squares contours $SS(\alpha, \beta)$ at the point $(\beta, \alpha) = (\beta_0, \alpha_0) = (0.02, 0.30)$. The center of the elliptical system is at $(\beta_1, \alpha_1) = (0.1007, 0.8416)$ and the next iteration begins from there. (*c*) Linearized sum of squares contours $SS(\alpha, \beta)$ at the point $(\beta, \alpha) = (\beta_1, \alpha_1) = (0.1007, 0.8416)$. The center of the elliptical system is at $(\beta_2, \alpha_2) = (0.1004, 0.3901)$ and the next iteration begins from there.

sum of squares as being based on approximately $44 - 2 = 42$ degrees of freedom (since two parameters have been estimated). In the nonlinear case this does not, in general, lead to an unbiased estimate of σ^2 as in the linear case, even when the model is correct.

A pure error estimate of σ^2 (see Section 2.1) can be obtained from the repeat observations. This provides a sum of squares $S_{pe} = 0.0024$ with 26 degrees of freedom.

An appropriate idea of possible lack of fit can be obtained by evaluating

$$S(\hat{\alpha}, \hat{\beta}) - S_{pe} = 0.0026 \quad \text{with} \quad 42 - 26 = 16 \text{ degrees of freedom}$$

and comparing the mean squares

$$\frac{(S(\hat{\alpha}, \hat{\beta}) - S_{pe})}{16} = 0.00016$$

$$\frac{S_{pe}}{26} = 0.00009.$$

An F-test is *not* applicable here but we can use the value of $F(16, 26, 0.95) = 2.08$ as a measure of comparison. We see that $16/9 = 1.8$, which would make us tentatively feel that the model does not fit badly.

Confidence Regions

We can calculate approximate $100(1 - q)\%$ confidence contours (described in Section 24.2) by finding points (α, β) that satisfy

$$\begin{aligned} S(\alpha, \beta) &= S(\hat{\alpha}, \hat{\beta}) \left[1 + \frac{p}{n - p} F(p, n - p, 1 - q) \right] \\ &= 0.0050[1 + F(2, 42, 1 - q)/21] \\ &= S_q. \end{aligned}$$

From Eq. (24.3.2) we can write this as

$$\sum_{u=1}^{n} \{(Y_u - 0.49e^{-\beta(X_u - 8)}) + \alpha(e^{-\beta(X_u - 8)} - 1)\}^2 = S_q$$

or

$$A\alpha^2 + 2B\alpha + C - S_q = 0,$$

where

$$A = \sum_{u=1}^{n} (e^{-\beta(X_u - 8)} - 1)^2,$$

$$B = \sum_{u=1}^{n} (Y_u - 0.49e^{-\beta(X_u - 8)})(e^{-\beta(X_u - 8)} - 1),$$

$$C = \sum_{u=1}^{n} (Y_u - 0.49e^{-\beta(X_u - 8)})^2$$

are all functions of β alone. We can thus select a value for q and then evaluate

$$\alpha = \frac{\{-B \pm [B^2 - A(C - S_q)]^{1/2}\}}{A}$$

for a range of β to obtain points on the boundaries of confidence regions with approximately $100(1 - q)\%$ confidence coefficients. The 75%, 95%, 99%, and 99.5% regions,

obtained from $q = 0.25, 0.05, 0.01$, and 0.005, respectively, are shown in Figure 24.8. The dot denotes the point $(\hat{\beta}, \hat{\alpha})$.

Points (β, α) that lie within the contour marked (say) 95% are considered, by the data, as not unreasonable for the true values of (β, α), at an approximate 95% level of confidence. The orientation and shape of the contours indicate that $\hat{\beta}$ is less well determined than $\hat{\alpha}$. (For discussion on this point in the linear case, see Section 24.5; see also Section 24.4.)

Some Typical Nonlinear Program Output Features

The printed output from nonlinear least squares programs varies from program to program. However, some features are common to many outputs and we now describe and illustrate these briefly, using the output from a Marquardt-type analysis of the example given in this section.

1. The *singular values* are the square roots of the eigenvalues of $\mathbf{Z}_j'\mathbf{Z}_j$, where $\mathbf{Z}_j$ is derived from Eq. (24.2.4) but employs the current $\boldsymbol{\theta}_j$ value and not $\boldsymbol{\theta}_0$. Widely disparate singular values indicate a tendency toward ill-conditioning. The corresponding singular vectors provide the orientation of the axes of the "linearization approximation bowl" with respect to the θ-axes.

Example 1. At $\hat{\theta}$ we have the following:

Singular values:	4.964	0.773
α:	−0.946	0.326
β:	0.326	0.946

The ratio of the largest and smallest singular values (there *are* only two singular values here, of course, but in general there would be p) is about 6.4, implying a fairly well-conditioned problem. (In an ill-conditioned problem, this ratio can be in the thousands. A ratio of 1 would imply circular linearizing approximating contours.) To achieve the same change in SS($\boldsymbol{\theta}$), one would have to move about 6.4 units in the β direction compared with one unit in the α direction. Reading down the columns, we see that the first singular direction

$$\phi_1 = -0.946\alpha + 0.326\beta$$

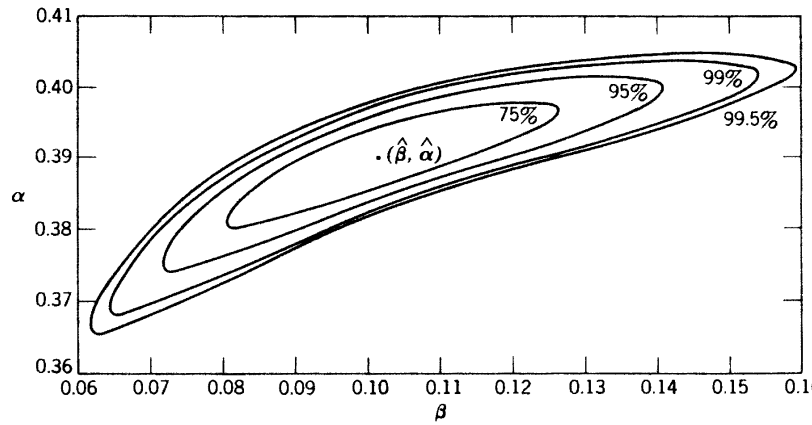

Figure 24.8. Confidence regions for (β, α). The regions are exact, the confidence levels approximate.

is mostly in the $-\alpha$ direction (the sign is not important here and is determined by the direction of the labeling only), while

$$\phi_2 = 0.326\alpha + 0.946\beta$$

is mostly in the β direction, as Figure 24.8 confirms should be the case. Note that the sum of squares of the coefficients (e.g., -0.946 and 0.326) is 1, apart from rounding error, and this sort of result is true in general for all the columns.

2. The *normalizing elements* are the square roots of the diagonal entries of the $\mathbf{Q} = ((q_{il})) = (\mathbf{Z}_j'\mathbf{Z}_j)^{-1}$ matrix. The linearized approximate *correlation matrix* $\mathbf{C} = ((c_{il}))$ of the $\hat{\theta}$'s is obtained by dividing each row and column of $(\mathbf{Z}_j'\mathbf{Z}_j)^{-1}$ by the two corresponding normalizing elements, which correspond to that row and column, namely, $c_{il} = q_{il}/(q_{ii}q_{ll})^{1/2}$.

Example 2.

Parameter:	α	β
Normalizing elements:	0.462	1.226
Parameter: α	1.000	
β	0.888	1.000

The correlation between α and β is positive, indicating that variations in (α, β) from $(\hat{\alpha}, \hat{\beta})$ in such a way that *both* increase, or *both* decrease, will give roughly similar SS($\boldsymbol{\theta}$) values. We can see from the $S(\alpha, \beta)$ plot (Figure 24.8) how this can happen. [Remember that the SS($\boldsymbol{\theta}$) ellipses around $\hat{\boldsymbol{\theta}}$ will mimic the $S(\boldsymbol{\theta})$ contours but not represent them perfectly.] Although 0.888 is a high correlation, it is not high enough for us to feel that the model is overparameterized. (For more on this point, see the "overparameterization" subsection, below.)

3. Confidence limits for the true values of the θ's can be evaluated on the basis of the linearized approximation, evaluated at $\hat{\boldsymbol{\theta}}$. The limits are, typically, $\hat{\theta}_i \pm 2\,\text{se}(\hat{\theta}_i)$, where $\text{se}(\hat{\theta}_i) = \{\text{appropriate diagonal element of } (\hat{\mathbf{Z}}'\hat{\mathbf{Z}})^{-1}s^2\}^{1/2}$, where $\hat{\mathbf{Z}}$ is the $\mathbf{Z}$ of Eq. (24.2.4) with $\hat{\boldsymbol{\theta}}$ replacing $\boldsymbol{\theta}_0$ and $s^2 = S(\hat{\boldsymbol{\theta}})/(n-p)$. These are, roughly, 95% limits in general.

Example 3.

	Lower Limit	Final Value	Upper Limit
α	0.380	0.390	0.400
β	0.075	0.102	0.128

The final estimate of α is $\hat{\alpha} = 0.390$ and an approximate 95% confidence band for α is (0.380, 0.400). The final estimate of β is $\hat{\beta} = 0.102$ with an approximate 95% confidence band for β of (0.075, 0.128). Note that the message implied by the width of the bands is confirmed by Figure 24.8. (The reader may wish to reread Section 5.4. Not only is the caution there valid but also the confidence statements made here apply only to the extent that the linearized model is a reliable approximation to the nonlinear model.) Both bands exclude zero, indicating nonzero values for α and β.

Curvature Measures

How close to reality is a linearized form of the nonlinear model in providing confidence statements on the parameters? The answer varies from problem to problem in a complicated way. Useful measures are described in Chapter 7 of Bates and Watts

(1988). These measures depend on second-order derivatives of the model function. A distinction can be made between *intrinsic nonlinearity* (which is dependent on the nature of the problem itself) and parameter effects nonlinearity (which may be reducible by a better choice of the parameterization—*if* a good choice can be found). A study of 67 specific data–model combinations with real sets of data, many of which are from "Exercises for Chapter 24" (H, L, M, N, and P), brought Bates and Watts to the following conclusions (their p. 256):

1. "Intrinsic curvature is smaller, and in almost all cases very much smaller, than the parameter effects curvature."
2. "Parameter effects curvatures . . . are often bad."
3. "Linear approximation inference regions . . . can be very misleading in many practical situations."

We do not explore these complications here and recommend the reference cited to readers with deeper interest in these topics. Many readers will find the usual linearized approximations perfectly adequate for making decisions on a day-to-day basis. Those who are involved in larger projects, or in a deep exploration of a specific few sets of data, may wish to delve further. In any event, mastery of the topics we have already dealt with is a prerequisite for moving on.

Overparameterization

Situations in which there are more parameters in the model than are needed to represent the data generally show up in the pattern of the (linearized) correlation matrix of the estimated coefficients. This matrix is given by taking $(\hat{\mathbf{Z}}'\hat{\mathbf{Z}})^{-1}$ and dividing the element in the ith row and jth column by

$$\{[i\text{th diagonal entry of } (\hat{\mathbf{Z}}'\hat{\mathbf{Z}})^{-1}] \times [j\text{th diagonal entry of } (\hat{\mathbf{Z}}'\hat{\mathbf{Z}})^{-1}]\}^{1/2},$$

which reduces the diagonal entries to 1's and the off-diagonal entries to correlations. When some of these correlations are large, it indicates that one or more parameters may not be useful or, more accurately, that a reparameterized model involving fewer parameters might do almost as well. Note that this does *not* necessarily mean that the original model is inappropriate for the physical situation under study. It may simply be an indication that the data in hand are not adequate to the task of estimating all the original parameters. (For example, in a linear model, when a parameter β does not appear to be different from zero, it does not always imply that the corresponding X is ineffective; it may be that, *in the particular set of data under study,* X does not change enough for its effect to be discernible. Similar, but more complicated, parallels arise in nonlinear work.)

In overparameterized situations, the $S(\boldsymbol{\theta})$ contours are often greatly elongated in the current $\boldsymbol{\theta}$-metric, and, in such cases, examination of an $S(\boldsymbol{\theta})$ plot, or sections of it according to the number of dimensions involved, can be very helpful.

24.4. A NOTE ON REPARAMETERIZATION OF THE MODEL

When the sum of squares surface, defined by Eq. (24.1.9), is attenuated and contains long ridges, slow convergence of any iterative estimation procedure is likely. As a

simple example of attenuation in the *linear* case, consider the model $Y_u = \theta_0 + \theta_1 X_u + \epsilon_u$ and suppose we have three observations Y_1, Y_2, and Y_3 at $X = 9$, 10, and 11. Then

$$\begin{aligned} S(\boldsymbol{\theta}) &= (Y_1 - \theta_0 - 9\theta_1)^2 + (Y_2 - \theta_0 - 10\theta_1)^2 + (Y_3 - \theta_0 - 11\theta_1)^2 \\ &= \sum_{u=1}^{3} Y_u^2 - 2\theta_0 \sum_{u=1}^{3} Y_u - 2\theta_1(9Y_1 + 10Y_2 + 11Y_3) \\ &\quad + 3\theta_0^2 + 302\theta_1^2 + 60\theta_0\theta_1. \end{aligned}$$

In coordinates (θ_0, θ_1), the contours of $S(\boldsymbol{\theta}) =$ constant are long thin ellipses. Such a sum of squares surface can be called *poorly conditioned* or ill-conditioned. However, if we rewrite the model as

$$\begin{aligned} Y_u &= (\theta_0 + \theta_1 \bar{X}) + \theta_1(X_u - \bar{X}) + \epsilon_u \\ &= \phi_0 + \phi_1 x_u + \epsilon_u, \end{aligned}$$

where $\phi_0 = \theta_0 + \theta_1 \bar{X}$, $\phi_1 = \theta_1$, $x_u = X_u - \bar{X}$ $(= -1, 0, 1$ for $u = 1, 2, 3)$, we obtain a sum of squares in terms of $\boldsymbol{\phi} = (\phi_1, \phi_2)'$ given by

$$\begin{aligned} S(\boldsymbol{\phi}) &= \sum (Y_u - \phi_0 - \phi_1 x_u)^2 \\ &= (Y_1 - \phi_0 + \phi_1)^2 + (Y_2 - \phi_0)^2 + (Y_3 - \phi_0 - \phi_1)^2 \\ &= \sum_{u=1}^{3} Y_u^2 - 2\phi_0 \sum_{u=1}^{3} Y_u + 2\phi_1(Y_1 - Y_3) + 3\phi_0^2 + 2\phi_1^2. \end{aligned}$$

In coordinates (ϕ_0, ϕ_1) these contours are "well-rounded" ellipses—the surface is said to be *well-conditioned.*

A similar sort of ill-conditioning can occur in nonlinear models of the form

$$Y_u = \theta_0 e^{\theta_1 X_u} + \epsilon_u$$

if the mean of the X_u, $\bar{X}$, is not close to zero. When expressions of this type occur it is sometimes better to consider the model in the alternative form

$$\begin{aligned} Y_u &= (\theta_0 e^{\theta_1 \bar{X}})(e^{\theta_1 (X_u - \bar{X})}) + \epsilon_u \\ &= \phi_0 e^{\phi_1 x_u} + \epsilon_u, \end{aligned}$$

where $\phi_0 = \theta_0 e^{\theta_1 \bar{X}}$, $\phi_1 = \theta_1$, and $x_u = X_u - \bar{X}$.

Note: In our example in Section 24.3 we did not do this. There it would have complicated the model since α occurred in two places and more than a simple replacement of one parameter by another is involved.

Suitable reparameterizations that will improve the conditioning of a sum of squares surface in a general case are not always apparent. Simple transformations that permit a "centering" of some variables, as in the examples above, may often be beneficial, however, and are often, at worst, harmless. For additional comments on reparameterization see the reference list at the end of the chapter.

24.5. THE GEOMETRY OF LINEAR LEAST SQUARES

There is a certain amount of overlap between this section (which has been preserved from the second edition) and the material in Chapters 20 and 21. However, the notation here is intended to conform more to what we need for Section 24.6, where the geometry

of nonlinear least squares is discussed. Sections 24.5 and 24.6 are self-contained and do not require Chapters 20 and 21 as prerequisite.

To understand why iterative methods applied to nonlinear problems are not always successful, it is helpful to consider the geometrical interpretation of *linear* least squares first of all. In the linear case, in the notation of this chapter we can write the model as

$$\begin{aligned} Y &= f(\boldsymbol{\xi}, \boldsymbol{\theta}) + \epsilon \\ &= \theta_1 X_1 + \theta_2 X_2 + \cdots + \theta_p X_p + \epsilon \end{aligned}$$

where the X_i are functions of $\boldsymbol{\xi}$. If we have observations Y_u containing errors ϵ_u when the X_i take the values $X_{1u}, X_{2u}, \ldots, X_{pu}$, for $u = 1, 2, \ldots, n$, then we can write the model in the alternative form:

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\theta} + \boldsymbol{\epsilon},$$

where

$$\mathbf{Y} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} X_{11} & X_{21} & \cdots & X_{p1} \\ X_{12} & X_{22} & \cdots & X_{p2} \\ \vdots & \vdots & & \vdots \\ X_{1n} & X_{2n} & \cdots & X_{pn} \end{bmatrix}, \quad \boldsymbol{\theta} = \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_p \end{bmatrix}, \quad \boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}.$$

(Note that we can obtain a "β_0 term" in the model in this form by taking $X_{1u} = 1$ for $u = 1, 2, \ldots, n$.) The sum of squares surface in Eq. (24.1.9) can be written as

$$\begin{aligned} S(\boldsymbol{\theta}) &= \sum_{u=1}^{n} \left[Y_u - \sum_{i=1}^{p} \theta_i X_{iu} \right]^2 \\ &= (\mathbf{Y} - \mathbf{X}\boldsymbol{\theta})'(\mathbf{Y} - \mathbf{X}\boldsymbol{\theta}) \\ &= \mathbf{Y}'\mathbf{Y} - 2\boldsymbol{\theta}'\mathbf{X}'\mathbf{Y} + \boldsymbol{\theta}'\mathbf{X}'\mathbf{X}\boldsymbol{\theta}. \end{aligned}$$

If we differentiate this expression with respect to $\boldsymbol{\theta}$, set the result equal to $\mathbf{0}$, and write $\hat{\boldsymbol{\theta}}$ for θ, we obtain the normal *equations*

$$\mathbf{X}'\mathbf{X}\hat{\boldsymbol{\theta}} = \mathbf{X}'\mathbf{Y},$$

with solution, if $\mathbf{X}'\mathbf{X}$ is nonsingular, given by

$$\hat{\boldsymbol{\theta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}.$$

We recall that the regression sum of squares is $\hat{\boldsymbol{\theta}}'\mathbf{X}'\mathbf{Y}$ and the residual sum of squares is $\mathbf{Y}'\mathbf{Y} - \hat{\boldsymbol{\theta}}'\mathbf{X}'\mathbf{Y}$. Now

$$\begin{aligned} S(\hat{\boldsymbol{\theta}}) &= \mathbf{Y}'\mathbf{Y} - 2\hat{\boldsymbol{\theta}}'\mathbf{X}'\mathbf{Y} + \hat{\boldsymbol{\theta}}'\mathbf{X}'\mathbf{X}\hat{\boldsymbol{\theta}} \\ &= \mathbf{Y}'\mathbf{Y} - \hat{\boldsymbol{\theta}}'\mathbf{X}'\mathbf{Y} - \hat{\boldsymbol{\theta}}'(\mathbf{X}'\mathbf{Y} - \mathbf{X}'\mathbf{X}\hat{\boldsymbol{\theta}}) \\ &= \mathbf{Y}'\mathbf{Y} - \hat{\boldsymbol{\theta}}'\mathbf{X}'\mathbf{Y} \end{aligned}$$

since $\hat{\boldsymbol{\theta}}$ satisfies the normal equations. Thus $S(\hat{\boldsymbol{\theta}})$, the smallest value of $S(\boldsymbol{\theta})$, is equal to the residual sum of squares in the analysis of variance table. We can also write

$$\begin{aligned} S(\boldsymbol{\theta}) - S(\hat{\boldsymbol{\theta}}) &= \boldsymbol{\theta}'\mathbf{X}'\mathbf{X}\boldsymbol{\theta} - 2\boldsymbol{\theta}'\mathbf{X}'\mathbf{Y} + \hat{\boldsymbol{\theta}}'\mathbf{X}'\mathbf{X}\hat{\boldsymbol{\theta}} \\ &= (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})'\mathbf{X}'\mathbf{X}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}). \end{aligned}$$

If the errors ϵ_u are independent and each follows the distribution $N(0, \sigma^2)$; that is, if

$\boldsymbol{\epsilon} \sim N(\mathbf{0}, \mathbf{I}\sigma^2)$, then it can be shown that, if the model is correct, the following results are true:

1. $\hat{\boldsymbol{\theta}} \sim N[\boldsymbol{\theta}, (\mathbf{X}'\mathbf{X})^{-1}\sigma^2]$.
2. $S(\hat{\boldsymbol{\theta}}) \sim \sigma^2\chi^2_{n-p}$.
3. $S(\boldsymbol{\theta}) - S(\hat{\boldsymbol{\theta}}) \sim \sigma^2\chi^2_p$.
4. $S(\boldsymbol{\theta}) - S(\hat{\boldsymbol{\theta}})$ and $S(\hat{\boldsymbol{\theta}})$ are distributed independently so that the ratio

$$\frac{[S(\boldsymbol{\theta}) - S(\hat{\boldsymbol{\theta}})]/p}{S(\hat{\boldsymbol{\theta}})/(n-p)} \sim F(p, n-p).$$

The contours defined by $S(\boldsymbol{\theta}) =$ constant can be examined in two different but related ways. We can examine them in the *sample space* (in which the mechanism of linear least squares can best be understood) or in the *parameter space* [in which we concentrate on the contours of $S(\boldsymbol{\theta})$ alone]. We shall now discuss these two representations.

The Sample Space

The sample space is an n-dimensional space. The vector of observations $\mathbf{Y} = (Y_1, Y_2, \ldots, Y_n)'$ defines a vector $\overrightarrow{OY}$ from the origin O to the point Y with coordinates $(Y_1, Y_2, \ldots, Y_n)$. The $\mathbf{X}$ matrix has p column vectors, each containing n elements. The elements of the jth column define the coordinates $(X_{j1}, X_{j2}, \ldots, X_{jn})$ of a point X_j in the sample space and the jth column vector of $\mathbf{X}$ defines the vector $\overrightarrow{OX}_j$ in the sample space. The p vectors $\overrightarrow{OX}_1, \overrightarrow{OX}_2, \ldots, \overrightarrow{OX}_p$ define a subspace of p dimensions, called the *estimation space,* which is contained within the sample space. Any point of this subspace can be represented by the end point of a vector, which is a linear combination of the vectors defining the space—that is, which is a linear combination of the columns of $\mathbf{X}$, such as, for example, $\mathbf{X}\boldsymbol{\theta}$ where $\boldsymbol{\theta} = (\theta_1, \theta_2, \ldots, \theta_p)'$ is a $p \times 1$ vector. Suppose the vector $\mathbf{X}\boldsymbol{\theta}$ defines the point T. Then the squared distance YT^2 is given by

$$(\mathbf{Y} - \mathbf{X}\boldsymbol{\theta})'(\mathbf{Y} - \mathbf{X}\boldsymbol{\theta}) = S(\boldsymbol{\theta})$$

as defined earlier. Thus the sum of squares $S(\boldsymbol{\theta})$ represents, in the sample space, the squared distance of Y from a general point T of the estimation space. Minimization of $S(\boldsymbol{\theta})$ with respect to $\boldsymbol{\theta}$ implies finding that value of $\boldsymbol{\theta}$, say, $\hat{\boldsymbol{\theta}}$, which provides a point P (defined by the vector $\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\theta}}$) of the estimation space closest to the point Y. Geometrically, then, P must be the foot of the perpendicular from Y to the estimation space, that is, the foot of a line passing through Y and orthogonal to all the vectors defined by the columns of the $\mathbf{X}$ matrix. In terms of vectors from the origin, we can write

$$\begin{aligned}\mathbf{Y} &= \hat{\mathbf{Y}} + (\mathbf{Y} - \hat{\mathbf{Y}}) \\ &= \hat{\mathbf{Y}} + \mathbf{e},\end{aligned}$$

where $\mathbf{e}$ is the vector of *residuals.* The vector $\mathbf{Y}$ is thus divided into two orthogonal components: (1) $\hat{\mathbf{Y}}$, which lies entirely in the estimation space, and (2) $\mathbf{Y} - \hat{\mathbf{Y}} = \mathbf{e}$, the vector of residuals, which lies in what is called the *error space.* The error space is defined as the $(n - p)$-dimensional subspace that remains of the full n-dimensional space, after the p-dimensional estimation space has been defined. The estimation and

error spaces are thus orthogonal. We can confirm algebraically that $\hat{\mathbf{Y}}$ and $\mathbf{e}$ are orthogonal as follows:

$$\begin{aligned}\hat{\mathbf{Y}}'\mathbf{e} &= (\mathbf{X}\hat{\boldsymbol{\theta}})'(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\theta}}) \\ &= \hat{\boldsymbol{\theta}}'\mathbf{X}'(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\theta}}) \\ &= \hat{\boldsymbol{\theta}}'(\mathbf{X}'\mathbf{Y} - \mathbf{X}'\mathbf{X}\hat{\boldsymbol{\theta}}) \\ &= \mathbf{0}\end{aligned}$$

since $\hat{\boldsymbol{\theta}}$ satisfies the normal equations, thus causing the parentheses to vanish. The vector $\mathbf{e}$ is a vector $\vec{OR}$, say, from the origin O, with length $OR = YP$, and with OR parallel to PY.

If T is a general point of the estimation space and YP is orthogonal to the space, then

$$YT^2 = YP^2 + PT^2$$

or

$$S(\boldsymbol{\theta}) = S(\hat{\boldsymbol{\theta}}) + PT^2.$$

Thus the contours for which $S(\boldsymbol{\theta})$ = constant must be such that

$$PT^2 = S(\boldsymbol{\theta}) - S(\hat{\boldsymbol{\theta}}) = \text{a constant.}$$

In the sample space, then, the contours defined by $S(\boldsymbol{\theta})$ = constant consist of all points T such that PT^2 = constant, that is, points in the estimation space and of the form $\mathbf{X}\boldsymbol{\theta}$ that lie on a p-dimensional sphere centered at the point P defined by $\mathbf{X}\hat{\boldsymbol{\theta}}$. The radius of this sphere is $[S(\boldsymbol{\theta}) - S(\hat{\boldsymbol{\theta}})]^{1/2}$. By using the fact, given earlier, that

$$\frac{[S(\boldsymbol{\theta}) - S(\hat{\boldsymbol{\theta}})]/p}{S(\hat{\boldsymbol{\theta}})/(n-p)} \sim F(p, n-p),$$

we can define the boundary of a $100(1-\alpha)\%$ confidence region for the point $\mathbf{X}\boldsymbol{\theta}$, which arises from the true (but unknown) value of $\boldsymbol{\theta}$, by

$$\frac{[S(\boldsymbol{\theta}) - S(\hat{\boldsymbol{\theta}})]/p}{S(\hat{\boldsymbol{\theta}})/(n-p)} = F(p, n-p, 1-\alpha),$$

that is, by

$$S(\boldsymbol{\theta}) = S(\hat{\boldsymbol{\theta}})\left[1 + \frac{p}{n-p}F(p, n-p, 1-\alpha)\right],$$

which is of the sensible form $S(\hat{\boldsymbol{\theta}})(1+q^2)$ indicating values of $S(\boldsymbol{\theta})$ somewhat greater than the minimum value $S(\hat{\boldsymbol{\theta}})$. The confidence region will thus consist of the inside of a sphere in the estimation space centered at P and with radius

$$[S(\boldsymbol{\theta}) - S(\hat{\boldsymbol{\theta}})]^{1/2} = \left[S(\hat{\boldsymbol{\theta}})\frac{p}{n-p}F(p, n-p, 1-\alpha)\right]^{1/2}.$$

The Sample Space When $n = 3$, $p = 2$

In order to illustrate the foregoing remarks by a diagram, we shall suppose that $n = 3$. When $n > 3$ the complete situation cannot be drawn but the mental extension to higher dimensions is not difficult.

Figure 24.9 shows the sample space when $n = 3$, the coordinate axes being labeled 1, 2, and 3 to correspond to the three components (Y_1, Y_2, Y_3) of the vector $\mathbf{Y}'$. We shall suppose that there are $p = 2$ parameters θ_1 and θ_2 so that $\mathbf{X}$ is a 3×2 matrix of form

$$\mathbf{X} = \begin{bmatrix} X_{11} & X_{21} \\ X_{12} & X_{22} \\ X_{13} & X_{23} \end{bmatrix}.$$

The columns of $\mathbf{X}$ define two points P_1 and P_2 with coordinates (X_{11}, X_{12}, X_{13}) and (X_{21}, X_{22}, X_{23}), respectively, and the vectors $\overrightarrow{OP}_1$ and $\overrightarrow{OP}_2$ define a plane that represents the two-dimensional estimation space in which the vector $\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\theta}}$ must lie. The point Y lies above this plane and the perpendicular YP from Y to the plane OP_1P_2 hits the plane at P. Thus YP is the shortest distance from Y to any point in the estimation space, P is defined by $\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\theta}}$, and $S(\hat{\boldsymbol{\theta}}) = YP^2$. In addition, since $OY^2 = \mathbf{Y}'\mathbf{Y}$, the standard analysis of variance breakup

$$\mathbf{Y}'\mathbf{Y} = \hat{\boldsymbol{\theta}}'\mathbf{X}'\mathbf{Y} + (\mathbf{Y}'\mathbf{Y} - \hat{\boldsymbol{\theta}}'\mathbf{X}'\mathbf{Y})$$

or

$$\mathbf{Y}'\mathbf{Y} = \hat{\boldsymbol{\theta}}'\mathbf{X}'\mathbf{Y} + S(\hat{\boldsymbol{\theta}})$$

is equivalent to the Pythagoras result:

$$OY^2 = OP^2 + YP^2.$$

If we draw a line OR through O, equal in length [so that $OR^2 = S(\hat{\boldsymbol{\theta}})$] and parallel to PY, then $\overrightarrow{OR}$ represents the vector of residuals $\mathbf{e} = \mathbf{Y} - \hat{\mathbf{Y}}$. The vector $\overrightarrow{OP}$ is $\hat{\mathbf{Y}}$

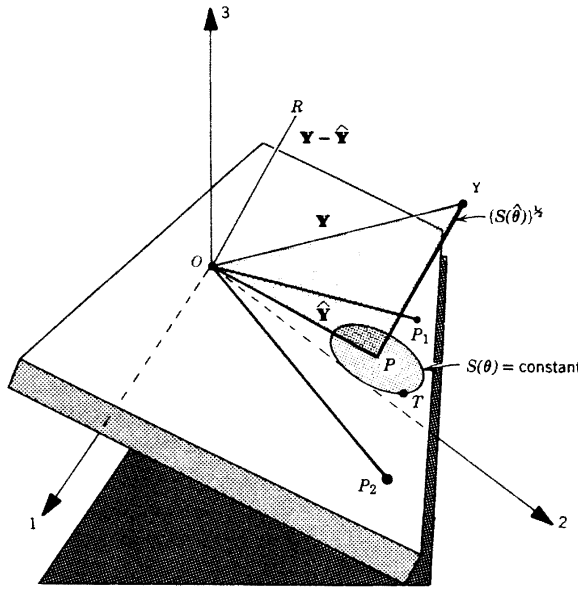

Figure 24.9. The sample space when $n = 3$, $p = 2$.

so we have the vector equation

$$\vec{OY} = \vec{OP} + \vec{OR}$$

or

$$\mathbf{Y} = \hat{\mathbf{Y}} + (\mathbf{Y} - \hat{\mathbf{Y}}).$$

We recall that, in general, contours of constant $S(\boldsymbol{\theta})$ are represented by p-dimensional spheres in the estimation space. Here, then, the contours must be circles on the plane OP_1P_2. This is easy to see, for if T is a general point $\mathbf{X}\boldsymbol{\theta}$ on the plane, $S(\boldsymbol{\theta})$ = constant means YT^2 = constant, so that $PT^2 = YT^2 - YP^2$ = constant. We thus obtain circles about P. One such circle is shown on the figure. The circle that provides a $100(1 - \alpha)\%$ confidence interval for the true point $\mathbf{X}\boldsymbol{\theta}$ has radius given by

$$[2S(\hat{\boldsymbol{\theta}})F(2, 1, 1 - \alpha)]^{1/2},$$

obtained by putting $n = 3, p = 2$ in the general formula.

The Sample Space Geometry When the Model Is Wrong

Suppose $\mathbf{Y} = \mathbf{X}\boldsymbol{\theta} + \boldsymbol{\epsilon}$ is the postulated linear model containing p parameters but that the true linear model is

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\theta} + \mathbf{X}_2\boldsymbol{\theta}_2 + \boldsymbol{\epsilon}$$

and contains additional terms $\mathbf{X}_2\boldsymbol{\theta}_2$ not considered. Then since the estimation space consists only of points of the form $\mathbf{X}\boldsymbol{\theta}$, the true point $\eta = \mathbf{X}\boldsymbol{\theta} + \mathbf{X}_2\boldsymbol{\theta}_2$ cannot lie in the estimation space. In this case the perpendicular YP from Y onto the estimation space (whose foot P is given by $\hat{\mathbf{Y}} = \mathbf{X}\boldsymbol{\theta}$) will be longer than it would have been if the correct model and estimation space had been used. To illustrate this point we shall give, in Figure 24.10, a diagram for the case $n = 3, p = 1$, where the true model contains two parameters θ and θ_2. The true model takes the form

$$\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix} = \begin{bmatrix} X_{11} \\ X_{12} \\ X_{13} \end{bmatrix} \theta + \begin{bmatrix} X_{21} \\ X_{22} \\ X_{23} \end{bmatrix} \theta_2 + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \end{bmatrix}$$

$$= \mathbf{X}\theta + \mathbf{X}_2\theta_2 + \boldsymbol{\epsilon}$$

and the postulated model is given when $\theta_2 = 0$. The single column of the $\mathbf{X}$ matrix defines the point P_1 and the line OP_1, which is the estimation space for the postulated model. The line YP is the perpendicular from Y onto OP_1 and P is the point $\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\theta}}$. Therefore the shortest squared distance $S(\hat{\theta})$, of all the squared distances $S(\theta)$ from the point Y to points $\mathbf{X}\theta$ on the line OP_1, is represented by the square of the length of YP. The true value of θ defines an unknown point $\mathbf{X}\theta$ on the line OP_1. A confidence interval for the true value $\mathbf{X}\theta$ can be constructed on OP_1 and around the point P.

Now the second vector $\mathbf{X}_2$ in the true model defines a line OP_2 and the lines OP_1 and OP_2 define a plane in which the true point $\mathbf{X}\theta + \mathbf{X}_2\theta_2$ lies. Suppose YP^* is the perpendicular from Y to the *correct* estimation space given by the plane OP_1P_2. Then P^* represents the point that would have given the correct fitted value $\hat{Y}^*$, say, *if* the correct model had been used. This is always of length less than or equal to YP since a perpendicular to a space (a plane here, OP_1P_2) cannot be longer than the

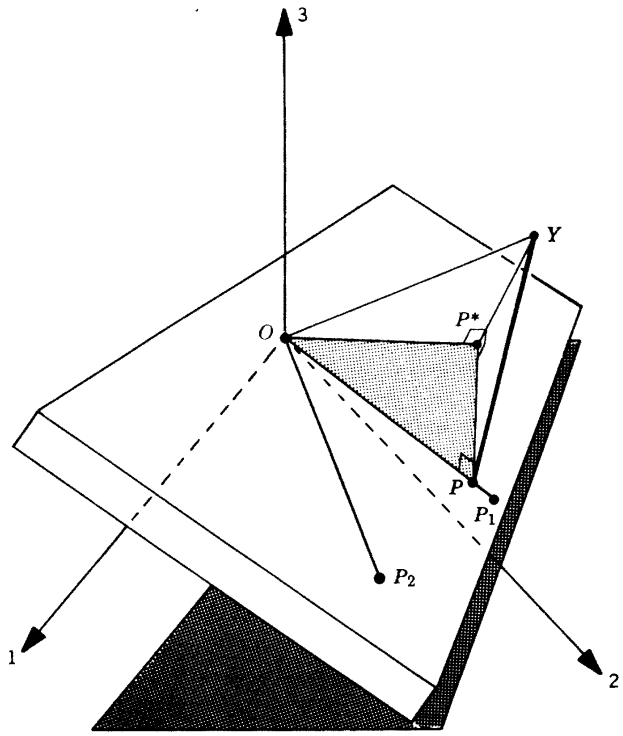

Figure 24.10. The sample space for $n = 3$, $p = 1$; wrong model.

perpendicular to an included space (here the line OP_1). If the model is incorrect, therefore, $S(\hat{\boldsymbol{\theta}}) = YP^2$ will be too long, if anything. [Note that it *could* happen that P and P^* coincide, so that the same minimum value $S(\hat{\boldsymbol{\theta}})$ would occur, whichever model was used. This would be very unusual, of course.]

When the postulated model is correct, in the general case, $S(\hat{\boldsymbol{\theta}})$ has expected or mean value $(n - p)\sigma^2$. If a pure error or prior estimate of σ^2 is available we know how big, roughly, the quantity YP^2 should be. However, if the postulated model is inadequate, YP^2 will probably be too long. The standard lack of fit test is thus examining the question: "Is the squared length YP^2 greater than we should expect on the basis of the good information we have about the size of the random error?" How much greater is *too great* is determined through the distribution properties involved, as formalized earlier.

Geometrical Interpretation of Pure Error

A geometrical interpretation of pure error is shown in Figure 24.11. In the sample space, O is the origin, Y is the end point of the vector $\mathbf{Y}$ of observations, and P is the foot of the perpendicular from Y onto the estimation space defined by the columns of the $\mathbf{X}$ matrix. Thus OP is the vector $\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\theta}}$. The point $\tilde{Y}$ is the end point of the vector $\tilde{\mathbf{Y}}$ whose ith element, $i = 1, 2, \ldots, n$, is

$$\tilde{Y}_i = (\text{average response in the group of repeats to which } Y_i \text{ belongs})$$
$$= \overline{Y}_{i0},$$

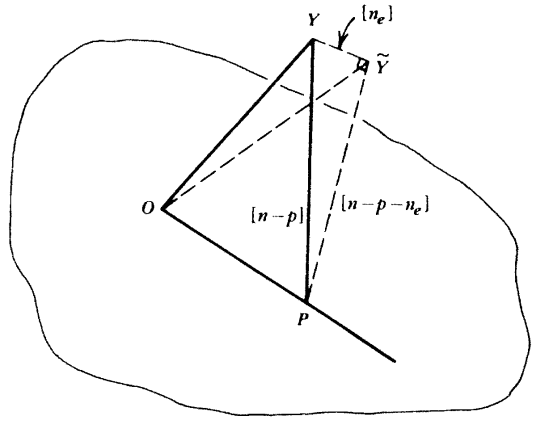

Figure 24.11. Geometrical representation of pure error. (The symbol $[n_e]$ means that the vector $\mathbf{Y} - \tilde{\mathbf{Y}}$, which is parallel to the line $Y\tilde{Y}$, lies in a subspace of the sample space of dimension n_e, etc.)

say. For nonrepeated points, $\overline{Y}_{i0} = Y_i$. It is easy to show that vectors $\mathbf{Y} - \tilde{\mathbf{Y}}$ and $\hat{\mathbf{Y}} - \tilde{\mathbf{Y}}$ are orthogonal so that the (respectively parallel) lines $Y\tilde{Y}$ and $\tilde{Y}P$ are perpendicular to each other, whereupon, by Pythagoras's theorem $Y\tilde{Y}^2 + \tilde{Y}P^2 = YP^2$. We can identify

YP^2 = squared length of residual vector $\mathbf{Y} - \mathbf{X}\boldsymbol{\theta}$ = residual sum of squares for the fitted model,
$Y\tilde{Y}^2$ = squared length of vector $\mathbf{Y} - \tilde{\mathbf{Y}}$ = pure error sum of squares,
$\tilde{Y}P^2$ = squared length of vector $\hat{\mathbf{Y}} - \tilde{\mathbf{Y}}$ = lack of fit sum of squares.

The F-test for lack of fit thus numerically compares $\tilde{Y}P^2/(n - p - n_e)$ with $Y\tilde{Y}^2/n_e$, where n_e is the pure error degrees of freedom and $(n - p - n_e)$ is the lack of fit degrees of freedom, each squared vector length being divided by the dimension of the subspace in which the corresponding vector lies. The F-distribution properties follow from the usual normality assumptions on the errors.

The Parameter Space

The parameter space is a p-dimensional space in which a set of values $(\theta_1, \theta_2, \ldots, \theta_p)$ of the parameters defines a point. The minimum value of $S(\boldsymbol{\theta})$ is attained at the point $\hat{\boldsymbol{\theta}} = (\hat{\theta}_1, \hat{\theta}_2, \ldots, \hat{\theta}_p)$. We recall that

$$S(\boldsymbol{\theta}) - S(\hat{\boldsymbol{\theta}}) = (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})'\mathbf{X}'\mathbf{X}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}).$$

All values of $\boldsymbol{\theta}$ that satisfy $S(\boldsymbol{\theta})$ = constant = K are given by

$$(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})'\mathbf{X}'\mathbf{X}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}) = K - S(\hat{\boldsymbol{\theta}})$$

and it can be shown that this is the equation of a closed ellipsoidal contour surrounding the point $\hat{\boldsymbol{\theta}}$. When $K_1 > K_2$ the contour $S(\boldsymbol{\theta}) = K_1$ completely encloses the contour $S(\boldsymbol{\theta}) = K_2$ and $\hat{\boldsymbol{\theta}}$ lies in the center of these nested p-dimensional "eggs." A $100(1 - \alpha)\%$ confidence region for the true (but unknown) value of $\boldsymbol{\theta}$ is enclosed by the contour, which is such that

$$\frac{[S(\boldsymbol{\theta}) - S(\hat{\boldsymbol{\theta}})]/p}{S(\hat{\boldsymbol{\theta}})/(n - p)} = F(p, n - p, 1 - \alpha)$$

if the errors are normally distributed, that is, $\boldsymbol{\epsilon} \sim N(\mathbf{0}, \mathbf{I}\sigma^2)$. This can be rearranged as

$$S(\boldsymbol{\theta}) = S(\hat{\boldsymbol{\theta}}) \left\{ 1 + \frac{p}{n-p} F(p, n-p, 1-\alpha) \right\}$$

in which the expression on the right-hand side is the constant value that defines the contour.

The Parameter Space When $p = 2$

We again use a simple case to illustrate the situation. Figure 24.12 shows some possible contours of the form $S(\boldsymbol{\theta}) =$ constant for three values of the constant when $p = 2$. The outer contour is labeled as a $100(1 - \alpha)\%$ confidence contour, defined as above. In the two-dimensional space of (θ_1, θ_2), the contours are concentric ellipses about the point $(\hat{\theta}_1, \hat{\theta}_2)$. Note that contours of this type are obtained no matter what the value of n (the number of observations) may be, since the dimension of the parameter space depends on p alone.

In general, the orientation and the shape of the ellipses are both of importance. If the axes of the ellipses are parallel to the θ_1 and θ_2 axes, then the value $\hat{\theta}_1$ that makes $S(\theta_1, \theta_2)$ a minimum has no dependence on θ_2; that is, if we fix θ_2 at any value the same value of $\theta_1 = \hat{\theta}_1$ minimizes $S(\theta_1, \theta_2 \mid \theta_2 \text{ fixed})$. This means that specific information about θ_2, which fixed its value, would not alter the least squares estimate $\hat{\theta}_1$. This situation occurs when the expression for $S(\theta_1, \theta_2)$ can be written without a cross-product term in $\theta_1\theta_2$. The model when $p = 2$ can be written as

$$Y_u = \theta_1 X_{1u} + \theta_2 X_{2u} + \epsilon_u, \qquad u = 1, 2, \ldots, n.$$

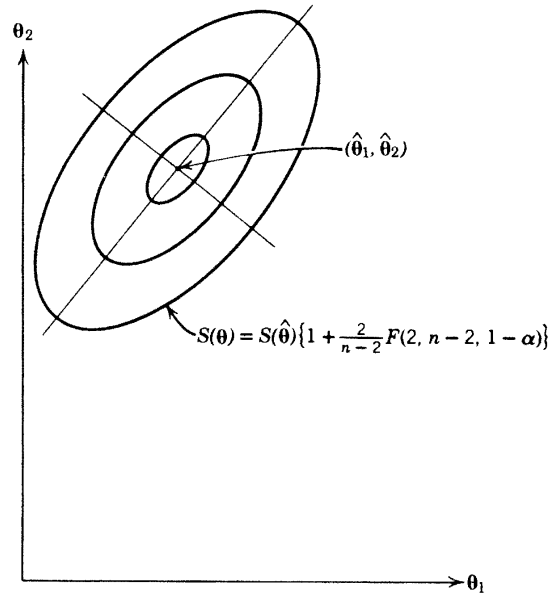

Figure 24.12. Contours of $S(\boldsymbol{\theta})$ in the parameter space when $p = 2$.

Thus

$$S(\boldsymbol{\theta}) = S(\theta_1, \theta_2) = \sum_{u=1}^{n} (Y_u - \theta_1 X_{1u} - \theta_2 X_{2u})^2$$
$$= \sum Y_u^2 - \theta_1 2 \sum X_{1u} Y_u - \theta_2 2 \sum X_{2u} Y_u$$
$$+ \theta_1^2 \sum X_{1u}^2 + \theta_2^2 \sum X_{2u}^2 + \theta_1 \theta_2 2 \sum X_{1u} X_{2u},$$

where all summations are over $u = 1, 2, \ldots, n$. It is clear from this that the minimizing value of θ_1, namely, $\hat{\theta}_1$, which satisfies $\partial S(\boldsymbol{\theta})/\partial \theta_1 = 0$, will not depend on θ_2 (and vice versa) if the coefficient of $\theta_1 \theta_2$ vanishes; that is, if $\Sigma X_{1u} X_{2u} = 0$, when the columns of the $\mathbf{X}$ matrix are orthogonal.

When the X_1 and X_2 columns of the $\mathbf{X}$ matrix are not orthogonal, a $\theta_1 \theta_2$ term occurs in $S(\theta_1, \theta_2)$, and the ellipses are obliquely oriented with respect to the θ_1 and θ_2 axes.

The shape of the $S(\theta_1, \theta_2)$ contours shows the relative precisions with which the estimates $\hat{\theta}_1$ and $\hat{\theta}_2$ are determined. Figure 24.13 illustrates some of the possibilities. The single contour shown is intended to represent the 95% confidence region boundary, and the point $\hat{\boldsymbol{\theta}}$ with coordinates $(\hat{\theta}_1, \hat{\theta}_2)$ is the least squares estimate of $\boldsymbol{\theta}$, in each case.

24.6. THE GEOMETRY OF NONLINEAR LEAST SQUARES

The Sample Space

When the model is nonlinear rather than linear there is no $\mathbf{X}$ matrix in the linear model sense. While there is still an estimation space it is not one defined by a set of vectors and may be very complex. The estimation space (also called the *solution locus*) consists of all points with coordinates expressible as

$$\{f(\boldsymbol{\xi}_1, \boldsymbol{\theta}), f(\boldsymbol{\xi}_2, \boldsymbol{\theta}), \ldots, f(\boldsymbol{\xi}_n, \boldsymbol{\theta})\}.$$

Since the sum of squares function $S(\boldsymbol{\theta})$ still represents the square of the distance from the point $(Y_1, Y_2, \ldots, Y_n)$ to a point of the estimation space, minimization of $S(\boldsymbol{\theta})$ still corresponds geometrically to finding a point P of the estimation space nearest to Y. The sample space for a very simple nonlinear example involving only $n = 2$ observations Y_1 and Y_2 taken at $\boldsymbol{\xi} = \boldsymbol{\xi}_1$ and $\boldsymbol{\xi} = \boldsymbol{\xi}_2$, respectively, and a single parameter θ, is shown in Figure 24.14. The estimation space consists of the curved line that contains points

$$\{f(\boldsymbol{\xi}_1, \theta), f(\boldsymbol{\xi}_2, \theta)\}$$

as θ varies, where $\boldsymbol{\xi}_1$, $\boldsymbol{\xi}_2$ are fixed. Y has coordinates (Y_1, Y_2), and P is the point of the estimation space nearest to Y.

Figure 24.15 shows the sample space for an example involving $n = 3$ observations Y_1, Y_2, and Y_3 taken at $\boldsymbol{\xi} = \boldsymbol{\xi}_1, \boldsymbol{\xi}_2$, and $\boldsymbol{\xi}_3$, respectively, and two parameters θ_1 and θ_2. The curved lines indicate the coordinate systems of the parameters on the estimation space or solution locus, which consists of all points of the form

$$\{f(\boldsymbol{\xi}_1, \theta_1, \theta_2), f(\boldsymbol{\xi}_2, \theta_1, \theta_2), f(\boldsymbol{\xi}_3, \theta_1, \theta_2)\}$$

as θ_1 and θ_2 vary, where $\boldsymbol{\xi}_1$, $\boldsymbol{\xi}_2$, and $\boldsymbol{\xi}_3$ are fixed. Y has coordinates (Y_1, Y_2, Y_3) and P is the point of the estimation space nearest to Y. When we apply the linearization technique to nonlinear problems we are selecting a point of the estimation space $\boldsymbol{\theta}_0$, say, as new origin, defining a linearized estimation space in the form of the tangent

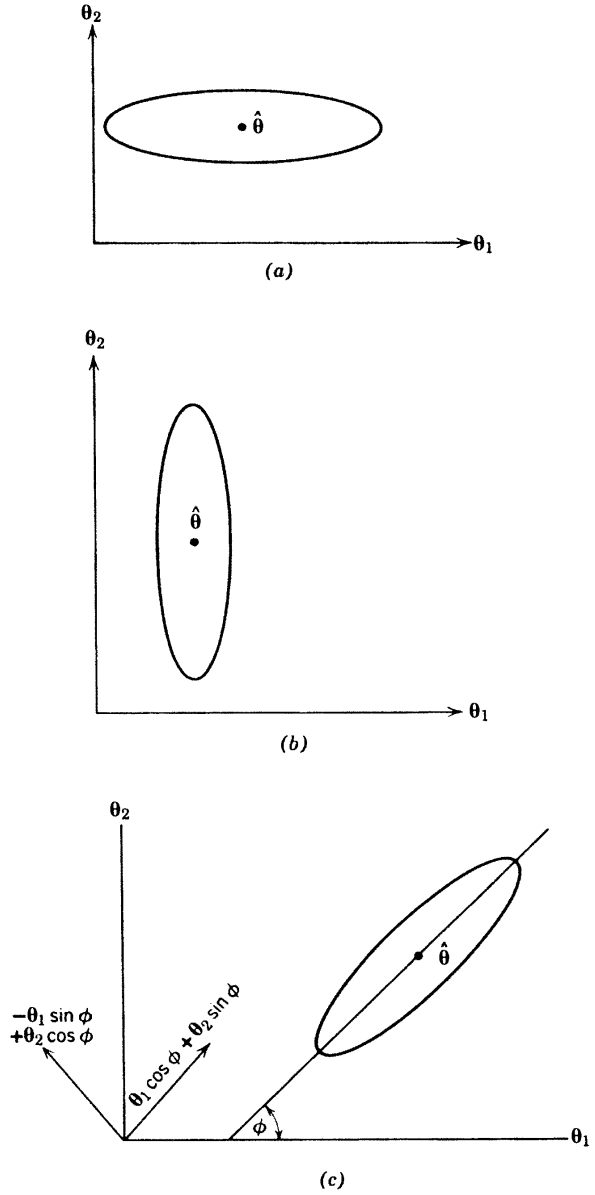

Figure 24.13. The interpretation of some possible 95% confidence regions for parameters (θ_1, θ_2). (*a*) $\hat{\theta}_1$ not well-determined; $\hat{\theta}_2$ well-determined; no dependence between $\hat{\theta}_1$ and $\hat{\theta}_2$. (*b*) $\hat{\theta}_1$ well-determined; $\hat{\theta}_2$ not well-determined; no dependence between $\hat{\theta}_1$ and $\hat{\theta}_2$. (*c*) $\hat{\theta}_1 \cos \phi + \hat{\theta}_2 \sin \phi$ not well-determined; $-\hat{\theta}_1 \sin \phi + \hat{\theta}_2 \cos \phi$ well-determined; dependence between $\hat{\theta}_1$ and $\hat{\theta}_2$.

space at $\boldsymbol{\theta}_0$ and solving the linearized least squares problem so defined. The solution to this (which will be given in units of rate of change of $\boldsymbol{\theta}$ that are appropriate at $\boldsymbol{\theta}_0$ only) are applied to the nonlinear problem, where they may not be correct, and another iteration is attempted. For a nonlinear problem involving only two observations and one parameter the effect will be as shown in Figure 24.16. Figure 24.16 shows the estimation space or solution locus with units of θ shown upon it. We assume here that $\theta_0 = 0$ and that the point marked $\theta = 1$ is the point of the estimation space attained

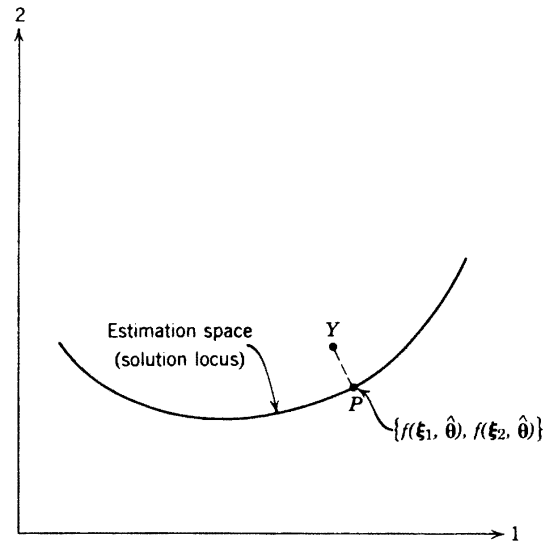

Figure 24.14. The sample space when $n = 2$, $f(\xi, \theta)$ nonlinear.

where $\theta = 1$, and so on. Note that the markings for θ are *not* equally spaced due to the nonlinearity and the nonuniformity of the coordinate system. The line tangent to the estimation space curve at $\theta = \theta_0 = 0$ is shown, graduated with units $\theta = 0, 1, 2, \ldots$, which are obtained from the rate of change found at θ_0. These units are equally spaced. We now find the least squares estimate of θ based on the linear assumption.

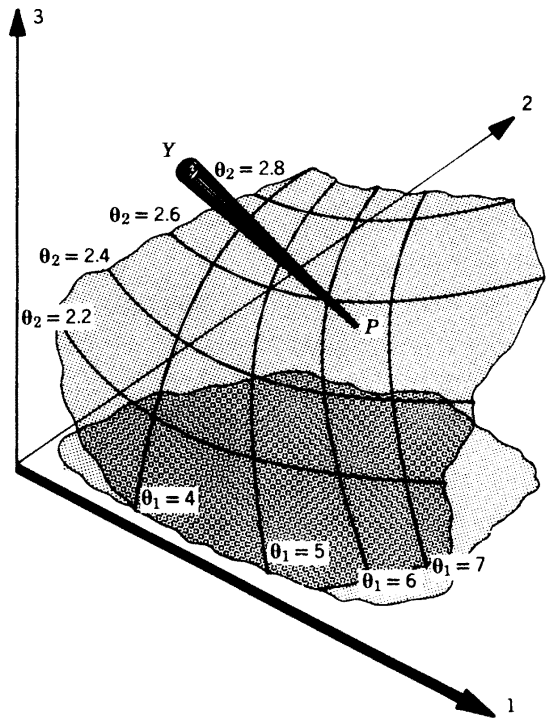

Figure 24.15. The sample space when $n = 3$, $p = 2$, $f(\xi, \theta)$ nonlinear.

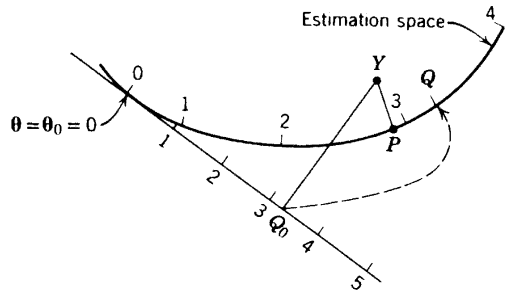

Figure 24.16. Geometrical interpretation of linearization method ($n = 2, p = 1$).

Geometrically, this means finding the point Q_0 so that YQ_0 is perpendicular to the tangent line. We see that, in the linearized units, a value of θ of about 3.2 (at Q_0) is indicated. In the next iteration of the linearization procedure we thus use the tangent line at the point where $\theta = 3.2$ on the *estimation space curve*, that is, at the point Q.

It is easy to see from this one reason why the linearization procedure sometimes fails. If the rate of change of $f(\boldsymbol{\xi}, \boldsymbol{\theta})$ is small at $\boldsymbol{\theta}_0$, but increases rapidly, the units on the tangent line may be quite unrealistic. For example, in Figure 24.17, the rate of change at $\theta_0 = 0$ is small and so the linearized units of θ are small. The actual units increase sharply, however. Thus, if we begin a further iteration using the indicated value of θ of about 26 at Q_0, our starting point on the estimation space will be farther from the best point P than was our original guess $\theta = \theta_0 = 0$. The situation may or may not be corrected in successive iterations. (Although we have used $\theta_0 = 0$ and units 1, 2, . . . , for simplicity, similar remarks apply in general whatever the value of the initial guess θ_0 and whatever the system of units near θ_0 may be.)

When there are more observations than two and more than one parameter the same ideas hold but the situation is more complicated and is difficult or impossible to draw.

When the model is linear, contours of constant $S(\boldsymbol{\theta})$ in the sample space consist of spheres. In nonlinear problems this is no longer true and quite irregular contours may

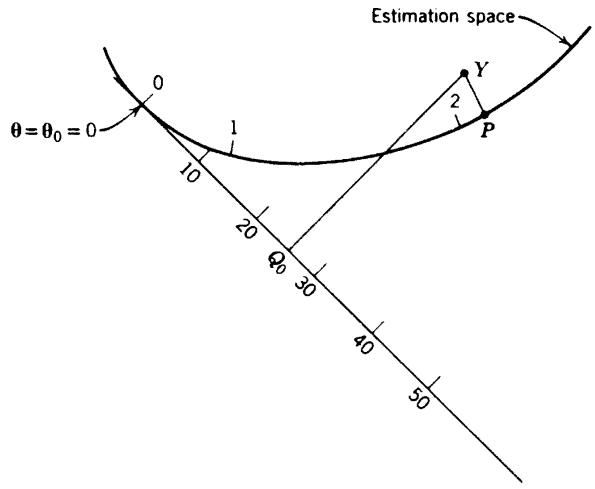

Figure 24.17. The effect on the linearization method of gross inequities in the systems of units ($n = 2, p = 1$).

arise consisting of all points of the estimation space equidistant, a selected distance, from the point $Y:(Y_1, Y_2, \ldots, Y_n)$.

The Parameter Space

In the linear model case, contours of constant $S(\boldsymbol{\theta})$ in the parameter space, or $\boldsymbol{\theta}$-space, consist of concentric ellipses. When the model is nonlinear the contours are sometimes banana-shaped, often elongated. Sometimes the contours stretch to infinity and do not even close, or they may have multiple loops surrounding a number of stationary values. When several stationary values exist they may have various levels or provide alternative minima for $S(\boldsymbol{\theta})$. Consider, for example, the model

$$Y = \frac{(\theta_1 e^{-\theta_2 t} - \theta_2 e^{-\theta_1 t})}{(\theta_2 - \theta_1)} + \epsilon.$$

Interchange of θ_1 and θ_2 leaves the model unaltered. Thus if the minimum $S(\boldsymbol{\theta})$ is attained at $(\theta_1, \theta_2) = (\hat{\theta}_1, \hat{\theta}_2)$, the same minimum value is given at $(\theta_1, \theta_2) = (\hat{\theta}_2, \hat{\theta}_1)$, so that a double solution exists. Multiple solutions are not easy to spot in this way in general. An example of banana-shaped contours is given in Section 24.3.

Confidence Contours in the Nonlinear Case

When the model is nonlinear a number of results that are true for the linear case no longer apply. When the error ϵ of the nonlinear model (24.1.5) is assumed to be normally distributed, $\hat{\boldsymbol{\theta}}$ is no longer normally distributed, $s^2 = S(\hat{\boldsymbol{\theta}})/(n - p)$ is no longer an unbiased estimate of σ^2, and there is no variance–covariance matrix of form $(\mathbf{X}'\mathbf{X})^{-1}\sigma^2$ in general.

Although confidence regions can still be *defined* by the expression

$$S(\boldsymbol{\theta}) = S(\hat{\boldsymbol{\theta}})\left\{1 + \frac{p}{n-p} F(p, n-p, 1-\alpha)\right\},$$

which provides a $100(1 - \alpha)\%$ confidence region in the linear model, normal error situation, the confidence coefficient will not be $1 - \alpha$, in the nonlinear case. We do not know in general what the confidence will be but we can call such regions *approximate* $100(1 - \alpha)\%$ *confidence regions* for $\boldsymbol{\theta}$. The banana-shaped regions for the example in Section 24.3 were obtained in this manner. While suitable comparisons of mean squares can still be made visually, the usual F-tests for regression and lack of fit are not valid, in general, in the nonlinear case.

Measuring Nonlinearity

Several suggestions have been made to meet the need for a measure of "the amount of nonlinearity" in nonlinear problems. Such a measure would help us decide when linearized results provide acceptable approximations, for example. For a brief discussion see the subsection "Curvature Measures" near the end of Section 24.3.

24.7. NONLINEAR GROWTH MODELS

This section is concerned with some examples of nonlinear models that have been used to describe growth behavior, as it varies in time. Growth models are applied in

many fields. In biology, botany, forestry, zoology, and ecology, growth occurs in organisms, plants, trees and bushes, animals, and human beings. In chemistry and chemical engineering, growth occurs as a result of chemical reactions. In economics and political science, growth of organizations, supplies of food and material, and nations occurs.

Types of Models

The type of model needed in a specific area and in a specific problem depends on the type of growth that occurs. In general, growth models are *mechanistic* rather than *empirical* ones. A mechanistic model usually arises as a result of making assumptions about the type of growth, writing down differential or difference equations that represent these assumptions, and then solving these equations to obtain a growth model. (An empirical model, on the other hand, is a model chosen to empirically approximate an unknown mechanistic model. Typically, the empirical model is a polynomial of some suitable order.)

An Example of a Mechanistic Growth Model

Consider a growth situation in which it is believed that the *rate* of growth at a particular time t is directly proportional to the amount of growth yet to be achieved. If we denote the limiting (i.e., the maximum possible) growth size by α, and if ω is the size at time t, then

$$\frac{d\omega}{dt} = k(\alpha - \omega), \tag{24.7.1}$$

where k is the *rate constant* of the growth pattern. Integrating Eq. (24.7.1) gives

$$\omega = \alpha(1 - \beta e^{-kt}), \tag{24.7.2}$$

usually known as the *monomolecular* growth function. This function rises steadily from a point $\alpha(1 - \beta)$ (at $t = 0$) to the limiting value of α. It has no point of inflection [i.e., there is no change in sign of the second derivative $(d^2\omega/dt^2)$ for any t], and it climbs steadily at a decreasing rate as in Eq. (24.7.1). It has been used in the past to represent the later portions of a life history (see, e.g., Gregory, 1928). Suppose we now wish to get some idea of what the curve described by Eq. (24.7.2) looks like. Because α is simply a scale factor, we can set $\alpha = 1$; also, because k and t only occur together as a unit, kt, we can take $k = 1$, for this purpose. Then, varying β, we get curves like those in Figure 24.18. Choice of a different value of α would change the vertical scale of the curve; choice of a different value of k would stretch out or contract the curve horizontally. Each curve starts at the value, when $t = 0$, of $\omega = \alpha(1 - \beta)$, which is simply $1 - \beta$ when $\alpha = 1$ as in Figure 24.18.

The curves drawn in Figure 24.18 are, of course, theoretical ones, based on the theoretical function given in Eq. (24.7.2). If we assume w_i, $i = 1, 2, \ldots, n$, to be observations of ω at times $t_1, t_2, \ldots, t_n$, we can postulate the model

$$w_i = \alpha(1 - \beta e^{-kt_i}) + \epsilon_i \tag{24.7.3}$$

where ϵ_i is a random error such that $E(\epsilon_i) = 0$, $V(\epsilon_i) = \sigma_i^2$, say. Suppose we assume that the errors ϵ_i all have the same variance and are uncorrelated. Then it is reasonable to use the least squares method to fit Eq. (24.7.3) to the data. Unless otherwise stated, we shall *always* assume our errors to be additive ones in the work that follows and

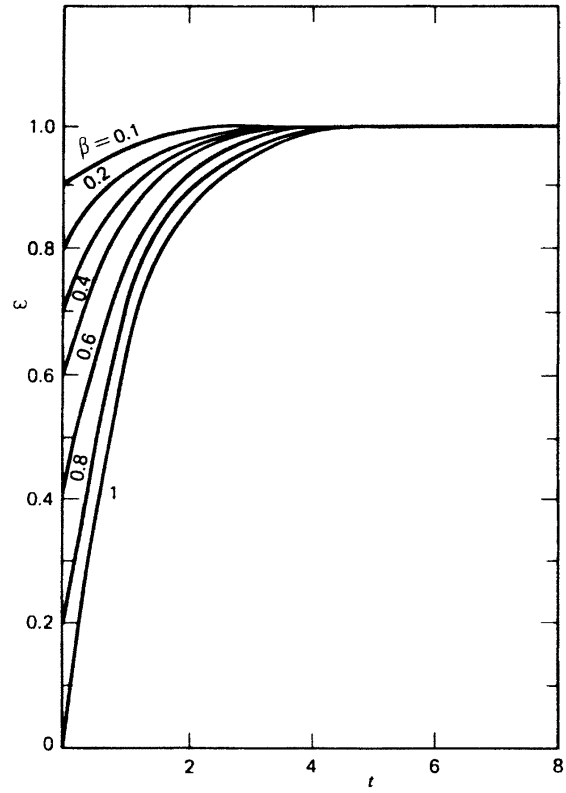

Figure 24.18. Theoretical curves of form $\omega = 1 - \beta e^{-t}$ for various β, as indicated.

will not repeat the above discussion. For example, "fitting the model given in Eq. (24.7.2)" will always mean use of Eq. (24.7.3), and so on for other models mentioned, unless otherwise specified.

Querying the Least Squares Assumptions

Growth data do not always satisfy the "usual least squares assumptions." For example, if the observations w_i are all taken on the same plant, animal, or organism, there is little reason to expect that they will be uncorrelated. Ideally, the experimenter should use different, independent items for each observation, but this is not always sensible or possible due to limitations on the experimental material or equipment. Also the $\sigma_i^2 = V(\epsilon_i)$ may well not all be the same and may depend, for example, on the growth size or some function of it. When specific information on such points is available, one can take advantage of it—for example, perhaps by using weighted least squares. Otherwise, the standard procedure is to fit the model in as common sense a manner as possible, and then to examine the residuals from the fit to see if they exhibit characteristics that give clues of invalid assumptions. These clues would then be used to iterate to an improved fitting procedure and/or an improved model.

The Logistic Model

Suppose the growth rate is such that (for $k > 0$)

$$\frac{d\omega}{dt} = \frac{k\omega(\alpha - \omega)}{\alpha}, \tag{24.7.4}$$

that is, it is proportional to the product of the present size and the future amount of growth, α being some limiting growth value. If we compare with Eq. (24.7.1) we see that it is now the growth rate *relative to present size*, $(d\omega/dt)/\omega$, that declines linearly with increasing ω. Integrating Eq. (24.7.4) we find

$$\omega = \alpha/\{1 + \beta e^{-kt}\}, \tag{24.7.5}$$

known as the *logistic* or *autocatalytic* growth function. This curve has an S-shape. Note that, for $t = 0$, $\omega = \alpha/(1 + \beta)$ so that this is the starting growth value; also, for $t = \infty$, $\omega = \alpha$, the limiting growth value. It follows that $\beta > 0$. Also it is clear that $k > 0$. From Eq. (24.7.4) it is obvious that the slope of the curve is always positive, and the second derivative,

$$\frac{d^2\omega}{dt^2} = \frac{k}{\alpha}(\alpha - 2\omega), \tag{24.7.6}$$

is positive for $\omega < \frac{1}{2}\alpha$, vanishes at the point of inflection where $\omega = \omega_I = \frac{1}{2}\alpha$, and is negative for $\omega > \frac{1}{2}\alpha$. At the point of inflection, substituting in Eq. (24.7.5), we find $t_I = (\ln \beta)/k$. Writing $t = t_I + u$ we can write Eq. (24.7.5) as $\omega = \alpha/(1 + e^{-ku})$ so that

$$\omega - \omega_I = \frac{\alpha}{2}\left\{\frac{1 - e^{-ku}}{1 + e^{-ku}}\right\} = g(u), \tag{24.7.7}$$

say, from which it is clear that the curve shape is symmetric about its point of inflection, because $g(-u) = -g(u)$. Of course, the curve extends only to $t = 0$ (i.e., $u = -t_I$) to the left, but to $t = \infty$ (i.e., $u = \infty$) to the right. Note that, if $0 < \beta < 1$, the curve begins *above* the point of inflection, while if β is very large and positive, the point of inflection is attained at a high value of t and may not appear in the t-range of the data. Of course, $\beta > 0$ because we must have $\alpha > \alpha/(1 + \beta)$.

To get some idea of how this family of curves looks, we can set $\alpha = 1$ without loss of generality and plot Eq. (24.7.5) for various β and k values. Some illustrative curves are shown in Figures 24.19 and 24.20. Changing β alters the starting point on the vertical scale at $t = 0$. Changing k alters the steepness of the curve. Of course, because

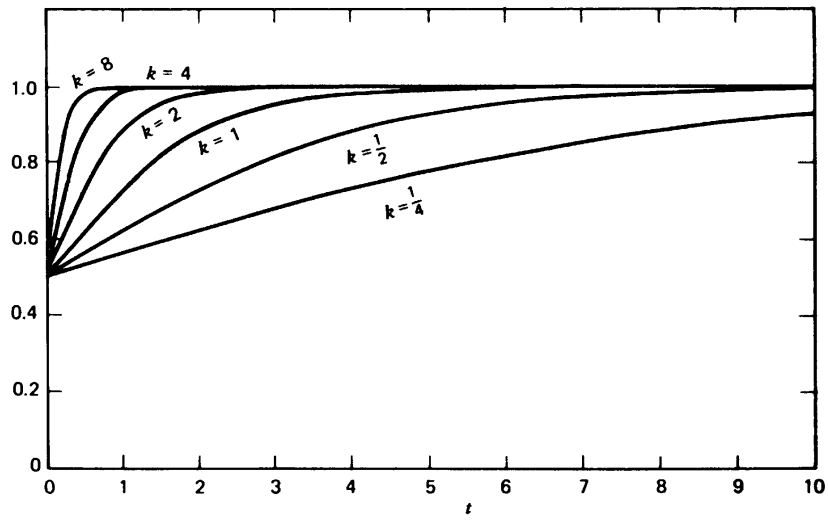

Figure 24.19. Theoretical curves of form $1/\{1 + e^{-kt}\}$ for various k, as indicated.

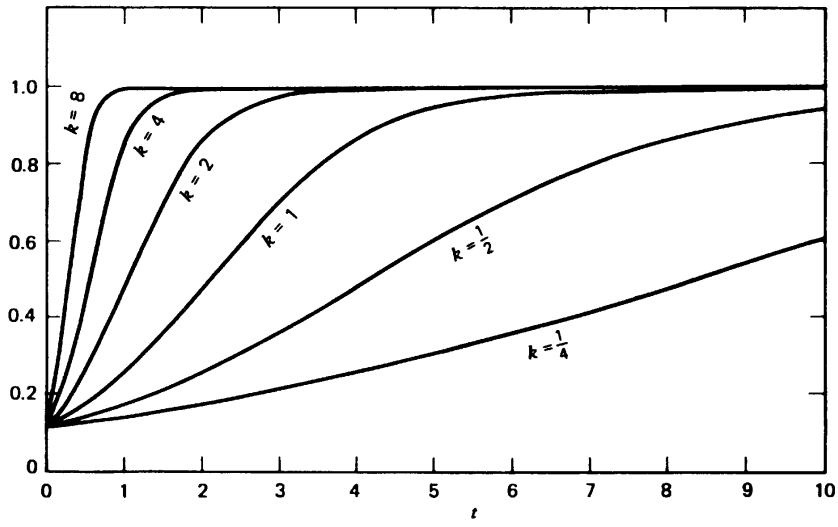

Figure 24.20. Theoretical curves of form $1/\{1 + 8e^{-kt}\}$ for various k, as indicated.

kt occurs as a product, a change of k can essentially be compensated by a recalibration of the t-axis; for example, $kt = (\frac{1}{2}k)(2t) = KT$, where $K = \frac{1}{2}k$ and $T = 2t$.

Another Form of the Logistic Model

Consider the model

$$\eta = \delta - \ln(1 + \beta e^{-kt}), \tag{24.7.8}$$

obtained by taking natural logarithms in Eq. (24.7.5), and setting $\eta = \ln \omega$ and $\delta = \ln \alpha$. Essentially, the curve shapes are similar to those of Figures 24.19 and 24.20 except that the vertical scale would be altered by the log transformation. Fitting Eqs. (24.7.5) and (24.7.8) by least squares involves completely different assumptions about the deviations from these models. According to Nelder (1961), the assumption that observations of η, $y_i = \ln w_i$, where the w_i are growth observations, have constant variance is usually a sensible one for the case of growing plants. In practice, both Eqs. (24.7.5) and (24.7.8) could be fitted and the residuals checked in both cases to see which model (if either) was suitable for the experimenter's purposes.

How Do We Get the Initial Parameter Estimates?

As we already know, nonlinear estimation procedures require initial parameter estimates and the better these initial estimates are, the faster will be the convergence to the fitted values. In fact, experience with growth models shows that, if the initial estimates are poor, convergence to the wrong final values can easily occur.

There is no general method for obtaining initial estimates. One uses whatever information is available. For example, for the logistic model (24.7.8), we can argue in this manner:

Step 1. When $t = \infty$, $\eta = \delta$. So take $\delta_0 = y_{\max}$.

Step 2. For any two other observations, the ith and jth, say, set

$$y_i = \delta_0 - \ln(1 + \beta_0 e^{-k_0 t_i}),$$
$$y_j = \delta_0 - \ln(1 + \beta_0 e^{-k_0 t_j}),$$

acting as though (24.7.8) were true without error for these observations. Then, developing, we find that

$$\exp(\delta_0 - y_i) - 1 = \beta_0 \exp(-k_0 t_i),$$
$$\exp(\delta_0 - y_j) - 1 = \beta_0 \exp(-k_0 t_j),$$

whereupon by division, taking natural logarithms, and rearrangement, we obtain

$$k_0 = \frac{1}{t_j - t_i} \ln \left\{ \frac{\exp(\delta_0 - y_i) - 1}{\exp(\delta_0 - y_j) - 1} \right\}.$$

In general i and j should be more widely spaced rather than otherwise, to lead to stable estimates.

Step 3. From the ith equation above we can evaluate

$$\beta_0 = \exp(k_0 t_i)\{\exp(\delta_0 - y_i) - 1\}.$$

(Either the ith or jth equation can be used; it makes no difference.)

Step 4. Substitution of $\delta_0 = y_{\max}$ in the two foregoing equations provides us with values for k_0 and β_0.

An alternative at the first step would be to take δ_0 somewhat bigger than $y_{\max}$, say, 110% of it, or whatever experience suggests. This would usually provide slightly better initial estimates. In some problems we can set $t = 0$ and set η at $t = 0$ to $y_{\min}$, or perhaps 90% of $y_{\min}$, and so on. In general, whatever method leads to simple equations to solve is employed to get the initial estimates.

Initial estimates for fitting the model (24.7.5) can similarly be obtained in the order α_0, k_0, β_0 from the equations

$$\alpha_0 = y_{\max},$$
$$\beta_0 = \{(\alpha_0 - w_i)/\alpha_0\}\exp(k_0 t_i),$$
$$k_0 = \frac{1}{t_i - t_j} \ln \left\{ \frac{\alpha_0 - w_j}{\alpha_0 - w_i} \right\}.$$

The Gompertz Model

If the growth rate

$$\frac{d\omega}{dt} = k\omega \log(\alpha/\omega), \tag{24.7.9}$$

we obtain, by integration, the Gompertz model

$$\omega = \alpha \exp\{-\beta e^{-kt}\}. \tag{24.7.10}$$

Although this curve is an S-shaped one like the logistic, it is not symmetrical about its point of inflection, the latter being where $d^2\omega/dt^2 = 0$, namely, where $\omega_I = \alpha/e =$

0.368α, which implies that $t_I = (\log \beta)/k$. Note that Eqs. (24.7.9) and (24.7.10) imply the relationships

$$\frac{d\omega/dt}{\omega} = k(\log \alpha - \log \omega), \tag{24.7.11}$$

$$\frac{d\omega/dt}{\omega} = k\beta e^{-kt}. \tag{24.7.12}$$

The latter can also be written as

$$\log\left\{\frac{d\omega/dt}{\omega}\right\} = \log(k\beta) - kt. \tag{24.7.13}$$

Thus Eq. (24.7.11) implies a linear relationship between the relative growth rate and $\log \omega$; Eq. (24.7.13) implies a linear relationship between the relative growth rate and time. According to Richards (1959), this curve has been used more for population studies and animal growth than for botanical applications; it was employed, for example, by Medawar (1940) in a study of the growth of a chicken's heart. It has also been applied, however, to the growth of *Pelargonium* leaves by Amer and Williams (1957).

As $t \to \infty$, $\omega \to \alpha$, the limiting growth. When $t = 0$, $\omega = \alpha e^{-\beta}$, the initial growth value. If, without loss of generality, we set $\alpha = 1$, we obtain, for $k = 1$ and selected β, the shapes shown in Figure 24.21. For each fixed value of β, variation in k produces sets of curves emanating from the same initial point, similar to the behavior shown in Figures 24.19 and 24.20 for the logistic model.

Von Bertalanffy's Model

This four-parameter model has the form

$$\omega = \{\alpha^{1-m} - \theta e^{-kt}\}^{1/(1-m)}, \tag{24.7.14}$$

where α, θ, k, and m are parameters to be estimated. In its original derivation by von Bertalanffy (1941, 1957) limits were imposed on m but Richards (1959) has pointed out its value over other ranges of m. Of special interest are these facts:

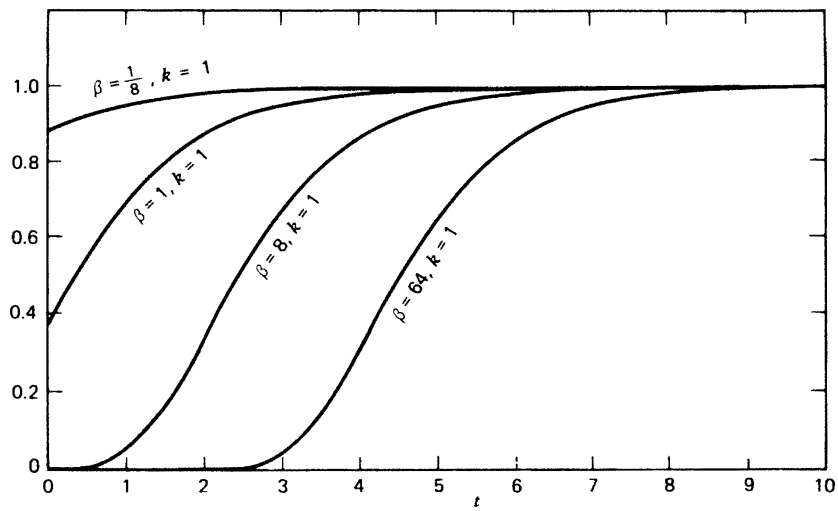

Figure 24.21. Selected theoretical curve forms of the Gompertz model $\omega = \alpha \exp(-\beta e^{-kt})$ for $\alpha = 1$.

1. When $m = 0$, we obtain the monomolecular function with a definition of $\theta = \alpha\beta$.
2. When $m = 2$, we obtain the logistic function with a definition of $\theta = \beta/\alpha$.
3. When $m \to 1$, the curve tends to the Gompertz form as can be shown by examining the limiting behavior of the growth rate, exact substitution leading to a breakdown. Thus estimated values of m close to 1 would indicate the usefulness of the Gompertz curve in a particular situation.
4. When $m > 1$, θ is negative; when $m < 1$, θ is positive.

Problems can arise when fitting this model if the current parameter values cause a negative quantity to be raised to a noninteger power and a constraint may have to be introduced to avoid this possibility in some cases. This can make the von Bertalanffy model somewhat awkward to fit compared with previous models.

24.8. NONLINEAR MODELS: OTHER WORK

Once we have methods of estimating the parameters of a nonlinear model (as earlier in this chapter) we can turn our attention to other problems. We discuss some important topics briefly and give references for further reading.

Design of Experiments in the Nonlinear Case

Reference. Box and Lucas (1959).

If we use the linearization method to estimate the parameters of a nonlinear model, we are led to the iterative formula

$$\mathbf{b}_j = (\mathbf{Z}_j' \mathbf{Z}_j)^{-1} \mathbf{Z}_j (\mathbf{Y} - \mathbf{f}^j)$$

to get $\boldsymbol{\theta}_{j+1} = \boldsymbol{\theta}_j + \mathbf{b}_j$. It can be shown that the approximate confidence region (see p. 516) at this stage for $\boldsymbol{\theta}$ has volume proportional to $|(\mathbf{Z}_j' \mathbf{Z}_j)^{-1}|$. Thus, if we regard the best design, that is, the best set of runs to take, as being the design that minimizes the volume of the confidence region, we need to

$$\text{Maximize } |\mathbf{Z}_j' \mathbf{Z}_j|.$$

How do we use this idea in practice?

If no runs have been performed, we choose the set of n runs (assume n is given) that

$$\text{Maximizes } |\mathbf{Z}_0' \mathbf{Z}_0|.$$

(Or, given several designs to choose from, we choose the one with the biggest $|\mathbf{Z}_0' \mathbf{Z}_0|$.)

If n runs have already been performed, and we wish to choose an $(n + 1)$st run, we can write down $|\mathbf{Z}_j' \mathbf{Z}_j|$ as a function of the $(n + 1)$st run and maximize $|\mathbf{Z}_j' \mathbf{Z}_j|$ with respect to the $(n + 1)$st run.

In general, this maximization has to be done numerically on a computer. Analytical solution is possible only in simple cases.

Example. Given $\boldsymbol{\theta}_0' = (\theta_{10}, \theta_{20}) = (0.7, 0.2)$ and the model

$$Y = \frac{\theta_1}{\theta_1 - \theta_2} \{ e^{-\theta_2 \xi} - e^{-\theta_1 \xi} \} + \epsilon,$$

select two runs ξ_1 and ξ_2 that maximize $|\mathbf{Z}_0'\mathbf{Z}_0|$. Differentiating $f(\theta_1, \theta_2, \xi)$ with respect to θ_1 and θ_2 and setting $\boldsymbol{\theta} = \boldsymbol{\theta}_0$ we obtain

$$Z_{1u}^0 = (0.8 + 1.4\xi_u)e^{-0.7\xi_u} - 0.8e^{-0.2\xi_u},$$

$$Z_{2u}^0 = -2.8e^{-0.7\xi_u} + (2.8 - 1.4\xi_u)e^{-0.2\xi_u}.$$

Thus

$$\mathbf{Z}_0 = \begin{bmatrix} Z_{11}^0 & Z_{21}^0 \\ Z_{12}^0 & Z_{22}^0 \end{bmatrix}.$$

Now here, $n = p = 2$. So we can write $|\mathbf{Z}_0'\mathbf{Z}_0| = |\mathbf{Z}_0'||\mathbf{Z}_0| = |\mathbf{Z}_0|^2$. So all we have to do in this case is to maximize

$$|\mathbf{Z}_0| = Z_{11}^0 Z_{22}^0 - Z_{12}^0 Z_{21}^0.$$

It can be shown numerically that this is a maximum when $\xi_1 = 1.23$, $\xi_2 = 6.86$, so that is our design. We would now find the Y-values at these two ξ's and go on to estimate θ_1 and θ_2 beginning with the initial estimates given, namely, (0.7, 0.2). For examples and discussion of the $n \to (n + 1)$ case see Box and Hunter (1965).

At stage n the experimenter would supply the computer with (1) the model, (2) the data, and (3) the current parameter estimates.

The computer would then produce:

1. The new least squares estimates.
2. The best conditions for the next experiment.
3. Information on the stability of the best conditions.
4. Any other items of special interest requested, for example, the covariance structure of the estimates.

A Useful Model-Building Technique

Reference. Box and Hunter (1962).

Suppose we wish to fit the model

$$Y = f(\theta_1, \theta_2, \ldots, \theta_p; W_1, W_2, \ldots, W_l) + \epsilon$$

$$= f(\boldsymbol{\theta}, \mathbf{W}) + \epsilon.$$

Let $X_1, X_2, \ldots, X_k$ be a set of predictor variables *not* in the model above. Write

$$X_{1j}, X_{2j}, \ldots, X_{kj} \text{ for the } j\text{th setting of these, } j = 1, 2, \ldots, n.$$

Suppose that, at each of these n settings, we have several runs with different sets of W's that we can estimate the parameters $\theta_1, \theta_2, \ldots, \theta_p$ at each of the n settings of the X's

This gives a table as follows:

					$\hat{\boldsymbol{\theta}}_i$				
					column				
X_{11}	X_{21}	X_{31}	$\cdots$	X_{k1}	$\hat{\theta}_{11}$	$\hat{\theta}_{21}$	$\cdots$	$\hat{\theta}_{i1}$	$\cdots$	$\hat{\theta}_{p1}$
X_{12}	X_{22}	X_{32}	$\cdots$	X_{k2}	$\hat{\theta}_{12}$	$\hat{\theta}_{22}$	$\cdots$	$\hat{\theta}_{i2}$	$\cdots$	$\hat{\theta}_{p2}$
$\vdots$	$\vdots$	$\vdots$		$\vdots$	$\vdots$	$\vdots$		$\vdots$		$\vdots$
X_{1n}	X_{2n}	X_{3n}	$\cdots$	X_{kn}	$\hat{\theta}_{1n}$	$\hat{\theta}_{2n}$	$\cdots$	$\hat{\theta}_{in}$	$\cdots$	$\hat{\theta}_{pn}$

We would expect each $\hat{\theta}_{ij}$ *column* to be "stable" if the X's had nothing to do with the response function. It follows that a way of checking whether the response function depends on the X's is to do a regression of the $\hat{\boldsymbol{\theta}}_i$ column on the set of X's and see if any regression coefficients are significant. That is, we fit the model

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_k X_k + \epsilon$$

or

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon},$$

where $\mathbf{Y} = \hat{\boldsymbol{\theta}}_i$, and $\mathbf{X}$ = the entire block of X's shown above. If the estimated coefficient of X_q is significantly different from zero, we conclude that the parameter θ_i depends on the variable X_q and so X_q should be in the original model. (So should any other X's whose coefficients are significant.) In other words, the original model $Y = f(\boldsymbol{\theta}, \mathbf{W}) + \epsilon$ is inadequate and needs reconsideration (see Figure 24.22).

For examples of the use of this technique when the X-values form a 2^{k-p} fractional factorial ($p \neq 0$) or a full factorial ($p = 0$) design see Hunter and Mezaki (1964) and Box and Hunter (1962).

Multiple Responses

References. Box and Draper (1965); Erjavec, Box, Hunter and MacGregor (1973); Bates and Watts (1988, Chapter 4).

In some situations, several response variables can be observed simultaneously and the models for these responses contain some or all of the same parameters. A good example of this is an "A goes to B goes to C" reaction with response functions

$$\eta_1 = \exp(-\phi_1 t),$$

$$\eta_2 = \{\exp(-\phi_1 t) - \exp(-\phi_2 t)\}\phi_1/(\phi_2 - \phi_1),$$

$$\eta_3 = 1 + \{-\phi_2 \exp(-\phi_1 t) + \phi_1 \exp(-\phi_2 t)\}/(\phi_2 - \phi_1),$$

all dependent on the predictor variable time (t) and one (η_1) or both of the parameters

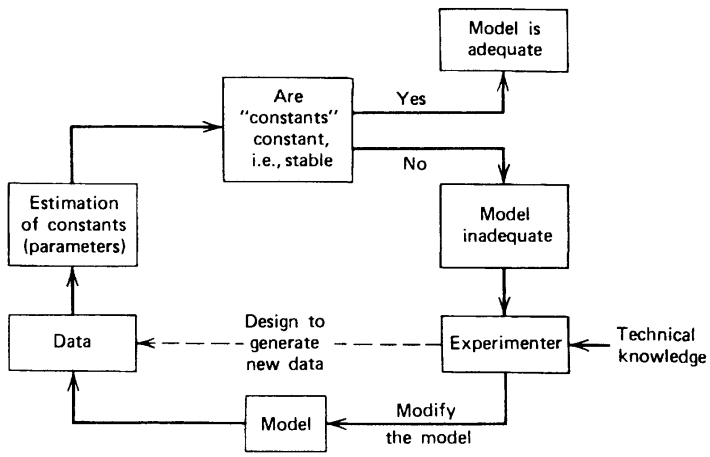

Figure 24.22. A diagrammatic representation of the adaptive model-building process. Adapted, with permission, from "A useful method of model building," by G. E. P. Box and W. G. Hunter, *Technometrics*, **4**, 1962, p. 302.

ϕ_1 and ϕ_2. Note that $\eta_1 + \eta_2 + \eta_3 = 1$ here; however, the corresponding observations (y_{1u}, y_{2u}, y_{3u}), $u = 1, 2, \ldots, n$, for (η_1, η_2, η_3) may be determined individually, in which case, $y_{1u} + y_{2u} + y_{3u}$ is not necessarily 1, due to random error. In such a case, the appropriate way of estimating the parameters is to minimize, with respect to those parameters, the determinant $\|v_{ij}\|$, where

$$v_{ij} = \sum_{u=1}^{n} (y_{iu} - \eta_{iu})(y_{ju} - \eta_{ju}),$$

are the sums of squares and the sums of products of the deviations of the observed y_{ij} from their respective models.

Problems can arise with this criterion when one or more of the responses is determined arithmetically from others. In our example, for instance, this would occur if y_{1u} and y_{2u} were actually measured but y_{3u} were determined as $1 - y_{1u} - y_{2u}$. Ways of detecting this, and of allowing for it, are discussed in the second reference mentioned above.

24.9. REFERENCES

Bates and Watts (1988); Bunke and Bunke (1989); Gallant (1987); Ratkowsky (1983, 1990); Ross (1990); Seber and Wild (1989).

EXERCISES FOR CHAPTER 24

A. Estimate the parameter θ in the nonlinear model

$$Y = e^{-\theta t} + \epsilon$$

from the following observations:

t	Y
1	0.80
4	0.45
16	0.04

Construct an approximate 95% confidence interval for θ.

B. Estimate the parameter θ in the nonlinear model

$$Y = e^{-\theta t} + \epsilon$$

from the following observations:

t	Y
0.5	0.96, 0.91
1	0.86, 0.79
2	0.63, 0.62
4	0.48, 0.42
8	0.17, 0.21
16	0.03, 0.05

Construct an approximate 95% confidence interval for θ.

C. Estimate the parameters α, β in the nonlinear model

$$Y = \alpha + (0.49 - \alpha)e^{-\beta(X-8)} + \epsilon$$

from the following observations:

X	Y
10	0.48
20	0.42
30	0.40
40	0.39

Construct an approximate 95% confidence region for (α, β).

D. The relationship between the yield of a crop, Y, and the amount of fertilizer, X, applied to that crop has been formulated as $Y = \alpha - \beta\rho^X + \epsilon$, where $0 < \rho < 1$. Given:

X	Y
0	44.4
1	54.6
2	63.8
3	65.7
4	68.9

obtain estimates of α, β, and ρ. Also construct an approximate 95% confidence region for (α, β, ρ).

E. The relationship between pressure and temperature in saturated steam can be written as

$$Y = \alpha(10)^{\beta t/(\gamma+t)} + \epsilon,$$

where

Y = pressure,
t = temperature,
α, β, γ = unknown constants.

The following data were collected:

t(°C)	Y(Pressure)
0	4.14
10	8.52
20	16.31
30	32.18
40	64.62
50	98.76
60	151.13
70	224.74
80	341.35
85	423.36
90	522.78
95	674.32
100	782.04
105	920.01

Obtain estimates of α, β, and γ. Also construct an approximate 95% confidence region for (α, β, γ).

F. Consider the model

$$Y = \theta + \alpha X_1 X_3 + \beta X_2 X_3 + \alpha\gamma X_1 + \beta\gamma X_2 + \epsilon.$$

Is this model nonlinear? How can estimates of the parameters be obtained by using only linear regression methods, if data $(Y_u, X_{1u}, X_{2u}, X_{3u})$ are available?

G. (*Source*: *Exploring the Atmosphere's First Mile,* Vol. 1, H. H. Lettau and B. Davidson, eds., Pergamon Press, New York, 1957, pp. 332–336.) Under adiabatic conditions, the wind speed Y is given by the nonlinear model

$$Y = \theta_1 \log(\theta_2 X + \theta_3) + \epsilon,$$

where

θ_1 = friction velocity (cm-sec^{-1}),

θ_2 = 1 + (zero point displacement)/(roughness length),

θ_3 = (roughness length)$^{-1}$ (cm^{-1}),

X = nominal height of anemometer (cm).

Estimate θ_1, θ_2, and θ_3 from the following data. Also construct an approximate 95% confidence region for $(\theta_1, \theta_2, \theta_3)$.

X	Y
40	490.2
80	585.3
160	673.7
320	759.2
640	837.5

H. (*Source*: "Planning experiments for fundamental process characterization," by W. G. Hunter and A. C. Atkinson, Technical Report No. 59, Statistics Dept., University of Wisconsin, Madison, Wisconsin, December 1965. For a shortened version of this paper see "Statistical designs for pilot-plant and laboratory experiments—Part II," *Chemical Engineering,* June 6, 1966, 159–164. The data originally appeared in "Kinetics of the thermal isomerization of bicyclo [2.1.1] hexane," by R. Srinivasan and A. A. Levi, *Journal of the American Chemical Society,* **85**, November 5, 1963, 3363–3365. Data on p. 3364 with "Reactant pressure, mm" values of less than unity have been omitted for the exercise.)

A certain chemical reaction can be described by the nonlinear model

$$Y = \exp\left\{-\theta_1 X_1 \exp\left[-\theta_2\left(\frac{1}{X_2} - \frac{1}{620}\right)\right]\right\} + \epsilon,$$

where θ_1 and θ_2 are parameters to be estimated, Y is the fraction of original material remaining, X_1 is the reaction time in minutes, and X_2 is the temperature in degrees Kelvin. Using the data below, which arose from an unplanned experiment, estimate θ_1 and θ_2 and construct a 95% confidence region for the point (θ_1, θ_2). You may use the preliminary estimates $\boldsymbol{\theta}_0' = (\theta_{10}, \theta_{20}) = (0.01155, 5000)$ if you wish.

Run	X_1	X_2	Y
1	120.0	600	0.900
2	60.0	600	0.949
3	60.0	612	0.886
4	120.0	612	0.785
5	120.0	612	0.791
6	60.0	612	0.890
7	60.0	620	0.787

Run	X_1	X_2	Y
8	30.0	620	0.877
9	15.0	620	0.938
10	60.0	620	0.782
11	45.1	620	0.827
12	90.0	620	0.696
13	150.0	620	0.582
14	60.0	620	0.795
15	60.0	620	0.800
16	60.0	620	0.790
17	30.0	620	0.883
18	90.0	620	0.712
19	150.0	620	0.576
20	60.0	620	0.802
21	60.0	620	0.802
22	60.0	620	0.804
23	60.0	620	0.794
24	60.0	620	0.804
25	60.0	620	0.799
26	30.0	631	0.764
27	45.1	631	0.688
28	40.0	631	0.717
29	30.0	631	0.802
30	45.0	631	0.695
31	15.0	639	0.808
32	30.0	639	0.655
33	90.0	639	0.309
34	25.0	639	0.689
35	60.1	639	0.437
36	60.0	639	0.425
37	30.0	639	0.638
38	30.0	639	0.659

I. (*Source*: See the Hunter and Atkinson reference in Exercise H.) Using the data below, which arose from a simulated planned experiment, estimate θ_1 and θ_2 in the model given in Exercise H and construct a 95% confidence region for (θ_1, θ_2). [It is interesting to note that the eight runs below, which were sequentially planned, produce a slightly smaller confidence region for (θ_1, θ_2) than the 38 unplanned experiments in Exercise H. This is a striking demonstration of the advantage of conducting planned experimentation whenever possible. Note particularly that the range of X_1 is now much greater than before. This, by itself, would lead to an improved confidence region if 38 unplanned runs were used. The planning of the experiment in addition makes it possible to use even fewer runs while maintaining about the same precision.]

Run	X_1	X_2	Y
1	109	600	0.912
2	65	640	0.382
3	1180	600	0.397
4	66	640	0.376
5	1270	600	0.342
6	69	640	0.358
7	1230	600	0.348
8	68	640	0.376

J. (*Source*: "Sequential design of experiments for nonlinear models," by G. E. P. Box and W. G. Hunter, *Proceedings of the IBM Scientific Computing Symposium on Statistics, October 21–23, 1963*, published in 1965, pp. 113–137). A certain chemical reaction can be described by the nonlinear model

$$Y = \theta_1\theta_3 X_1/(1 + \theta_1 X_1 + \theta_2 X_2) + \epsilon,$$

where Y is the reaction rate, X_1 and X_2 are partial pressures of reactant and product, respectively, θ_1 and θ_2 are adsorption equilibrium constants for reactant and product, respectively, and θ_3 is the effective reaction rate constant. Use the data below to estimate θ_1, θ_2, and θ_3 and construct a 95% confidence region for $(\theta_1, \theta_2, \theta_3)$. You may use the preliminary estimates $\boldsymbol{\theta}_0' = (\theta_{10}, \theta_{20}, \theta_{30}) = (2.9, 12.2, 0.69)$ if you wish. These data are reprinted by permission of International Business Machines Corporation.

Run	X_1	X_2	Y
1	1.0	1.0	0.126
2	2.0	1.0	0.219
3	1.0	2.0	0.076
4	2.0	2.0	0.126
5	0.1	0.0	0.186
6	3.0	0.0	0.606
7	0.2	0.0	0.268
8	3.0	0.0	0.614
9	0.3	0.0	0.318
10	3.0	0.8	0.298
11	3.0	0.0	0.509
12	0.2	0.0	0.247
13	3.0	0.8	0.319

K. (*Source*: *Statistical Theory with Engineering Applications*, by A. Hald, Wiley, New York, 1960 p. 564.) Fit, to the constructed representative data below, the nonlinear model

$$Y = \theta_1 X^{\theta_2} + \epsilon$$

and provide a 95% confidence region for the parameters (θ_1, θ_2). For a larger body of data, see the reference above.

Speed of Automobile X	Stopping Distance Y
4	5
10	20
17	45
22	66
25	85

L. (*Source*: "Biochemical oxygen demand data interpretation using the sum of squares surface," by Donald Marske, M.S. thesis in Civil Engineering, University of Wisconsin, Madison, Wisconsin, 1967.) Fit, to each set of data below, the nonlinear model

$$Y = \theta_1(1 - e^{-\theta_2 t}) + \epsilon$$

and provide an approximate 95% confidence region for (θ_1, θ_2).

Set 1:

t	Y
1	82
2	112
3	153
4	163
5	176
6	192
7	200

Set 2:

t	Y
1	0.47
2	0.74
3	1.17
4	1.42
5	1.60
7	1.84
9	2.19
11	2.17

Set 3:

t	Y
1	168
2	336
3	468
5	660
6	708
7	696

Set 4:

t	Y
1	9
2	9
3	16
4	20
5	21
7	22

Set 5:

t	Y
1	4.3
2	8.2
3	9.5
4	10.4
5	12.1
7	13.1

Set 6:

t	Y
1	6.8
2	12.7
3	14.8
4	15.4
5	17.0
7	19.9

Set 7:

t	Y
1	109
2	149
3	149
5	191
7	213
10	224

Set 8:

t	Y
1	8.3
2	10.3
3	19
4	16
5	15.6
7	19.8

Set 9:

t	Y
1	4710
2	7080
3	8460
4	9580

M. To the ice crystal data of Exercise 13E fit the nonlinear model $M = \alpha T^{\beta} + \epsilon$. Examine the residuals and state your conclusions.

N. The data below arose from five orange trees grown at Riverside, California, during the period 1969–1973. The response w in the body of the table is the trunk circumference in millimeters, and the predictor variable t is the time in days, with an arbitrary origin taken on December 31, 1968. Fit the models given in Eqs. (24.7.2), (24.7.5), (24.7.8), and (24.7.10) to these data. Based on a visual inspection of the fitted models, which seems to be most useful?

	Response w for Tree No.				
t	1	2	3	4	5
118	30	33	30	32	30
484	58	69	51	62	49
664	87	111	75	112	81
1004	115	156	108	167	125
1231	120	172	115	179	142
1372	142	203	139	209	174
1582	145	203	140	214	177

O. Estimate the parameters α, β in the nonlinear model $Y = \alpha + X^{\beta} + \epsilon$, using the data $(X, Y) = (0, -1.1), (1, 0), (2, 2.9), (3, 8.1)$. [This can be done either by (1) nonlinear least squares or (2) fixing β, setting $\hat{\alpha}(\beta) = \{\text{average of the } (Y_u - X_u^{\beta})\}$, the appropriate linear least squares estimate of α for specified β, plotting $S(\alpha, \beta) = \sum_{u=1}^{n} \{Y_u - \hat{\alpha}(\beta) - X_u^{\beta}\}^2$ versus β and estimating $\hat{\beta}$ as the value of β that minimizes $S(\alpha, \beta)$; the appropriate $\hat{\alpha}$ is then $\hat{\alpha}(\hat{\beta})$ the value of $\hat{\alpha}$ that corresponds to $\hat{\beta}$.]

P. Three tensile properties of ductile cast iron are

$$x = \text{percentage elongation},$$

$$y = \text{tensile strength, kg/in.}^2$$

and

$$z = \text{yield strength, kg/in.}^2$$

It has been suggested[1] that models of the form

$$y = \alpha + \beta/x^{\gamma} + \epsilon,$$

$$z = \delta + \theta/x^{\phi} + \epsilon$$

hold for these properties and that the model parameters might be suitable measures of the quality of the iron.

The figures in the table below represent minimum values of the qualities indicated, as given in a particular industry specification ASTM A53 6-70 to which ductile iron is manufactured. Fit the models above to these data and so obtain estimates of the parameters. [*Hint*: The two models are both linear in the transformed predictor variables $x^{-\gamma}$ and $x^{-\phi}$. For the first model, assume for the moment that γ is fixed. Then we can solve the least squares normal equations for $\hat{\alpha}$ and $\hat{\beta}$, both of which depend on γ and so write an expression, depending only on the unknown γ, for the sum of squares function

$$S(\gamma) = \sum_{u=1}^{n} (y_u - \hat{\alpha} - \hat{\beta}/x_u^{\gamma})^2.$$

By letting γ vary and plotting, or printing out a table of $S(\gamma)$, we find the $\hat{\gamma}$ that minimizes $S(\gamma)$. This $\hat{\gamma}$ and the corresponding $\hat{\alpha}$ and $\hat{\beta}$ are then the appropriate least squares estimators to use. The same idea is employed to get $\hat{\delta}$, $\hat{\theta}$, and $\hat{\phi}$.]

Percentage Elongation x	Tensile Strength, kg/in.^{2} y	Yield Strength, kg/in.^{2} z
2	120	90
3	100	70
6	80	55
12	65	45
18	60	40

Q. Fit the model $Y = \alpha X_1^{\beta} X_2^{\gamma} + \epsilon$ to the data of Exercise 13F.

R. (*Source*: "The utilization of dietary energy by steers during periods of restricted food intake and subsequent realimentation. Part 1," by H. P. Ledger and A. R. Sayers, *Journal of Agricultural Science, Cambridge*, **88**, 1977, 11–26. "Part 2," by H. P. Ledger is on pp. 27–33 of the same journal issue. Adapted with the permission of Cambridge University Press.)

[1]By C. R. Loper, Jr., and R. M. Kotschi of the University of Wisconsin to whom we are grateful for this exercise.

TABLE R. Group Mean Daily Dry Matter Intake as Percentage of Live Weight

Reference Designation of Data Set		Weeks on Maintenance							
		3	6	9	12	15	18	21	24
B 185 kg	%	1.835	1.255	1.037	1.045	0.900	0.901	0.836	0.896
	sd	0.412	0.315	0.692	0.712	0.149	0.197	0.156	0.234
B 275 kg	%	1.702	1.313	1.037	0.952	0.863	0.879	0.897	0.800
	sd	0.292	0.262	0.245	0.187	0.161	0.145	0.160	0.199
B × H 275 kg	%	1.545	1.134	0.941	0.840	0.791	0.822	0.855	0.773
	sd	0.206	0.205	0.215	0.211	0.293	0.095	0.072	0.124
¾ B 450 kg	%	0.999	0.803	0.790	0.797	0.734	0.687	0.687	0.716
	sd	0.287	0.191	0.168	0.093	0.127	0.145	0.162	0.224
¾ H 450 kg	%	0.818	0.753	0.737	0.713	0.664	0.660	0.706	0.670
	sd	0.249	0.185	0.133	0.140	0.196	0.122	0.122	0.114

The table shows values of the response Y = group mean daily dry matter intake as percentage of live weight of steers, measured at eight equally spaced values of X = weeks on maintenance. Also shown are the standard deviations (sd) of the Y's. There are five groups of such data, as designated in the left column. (Thus, for example, in the fourth group, the sixth response observation is $Y = 0.687$, with sd = 0.145, and $X = 18$.) To each group of data fit, by weighted least squares, the model

$$Y = \beta_0 + \beta_1 \theta^X + \epsilon,$$

and provide the usual analyses.

[*Hints*: If a weighted nonlinear least squares program is not available to you, the following approaches are possible:

1. Use weighted linear least squares over a selected range of values of θ (such as $0 \leq \theta \leq 1$) and estimate θ as the value that gives the smallest residual sum of squares. For that value of θ, estimate β_0 and β_1.
2. Write the model as

$$Y/\text{sd} = (1/\text{sd})\beta_0 + (\theta^X/\text{sd})\beta_1 + \text{error}$$

and use ordinary (unweighted) nonlinear least squares to estimate β_0, β_1, and θ.

3. Write the model as in (2) and use ordinary (unweighted) linear least squares over a selected range of values of θ (such as $0 \leq \theta \leq 1$) and estimate θ as the value that gives the smallest residual sum of squares. For that estimate of θ, estimate β_0 and β_1,

Note that $\mathbf{V}(\mathbf{Y})$ is a diagonal matrix in this problem.]

S. (*Source*: Carol C. House, U.S. Department of Agriculture, Washington, DC, 20250.) The data in the table consist of eight samples taken in a corn growth study, in which were measured:

Y = mean dry kernel weight of four plants,

t = mean time since silking of four plants.

1. Fit, to each individual sample, the nonlinear model

$$\ln Y = \delta - \ln(1 + \beta e^{-kt}) + \epsilon,$$

where δ, β, and k are parameters to be estimated from the data.

2. Plot each data sample and show the corresponding fitted curve on the same diagram. Comment on what you see, both in the diagrams and in the computer output.
3. Plot a dot diagram of all eight $\hat{\delta}$'s; do the same for the $\hat{\beta}$'s; and the $\hat{k}$'s. Comment on what you see in these plots. What would you *expect* to see, if there were no differences from sample to sample?
4. Fit the model in (1) to *all* the data at once and add the resulting parameter estimates to your dot diagrams in (3). What do you conclude?

5. The data values in the table are all means of four readings. If the individual readings that provided these means were available, would you use them in the model-fitting procedure instead of the means? Why or why not? Give the advantages and disadvantages.

Sample	Y	t	Sample	Y	t
8	11.44	13.625	24	37.84	18.625
	29.51	19.750		67.34	29.125
	69.05	28.625		157.10	49.250
	98.79	41.750	32	7.84	13.375
	138.01	49.625		15.12	16.875
	162.82	69.625		73.97	28.250
14	35.88	19.750		110.58	43.125
	106.89	30.250		114.36	47.500
	168.58	35.625		185.87	58.000
	136.84	43.375		115.18	60.625
	164.50	49.500	52	10.60	8.750
16	3.52	6.500		15.13	14.875
	10.56	14.875		38.74	22.500
	41.55	24.625		120.19	37.625
	94.55	35.875		126.32	41.750
	122.52	49.875		171.75	51.625
	130.19	56.875		156.67	63.875
22	14.26	17.125	54	11.92	13.625
	50.51	25.625		66.82	24.750
	60.83	29.625		28.29	24.875
	104.78	39.625		106.92	39.000
	96.46	46.375		129.83	53.875
	97.02	54.250		143.26	60.875
	172.41	62.125			

T. (*Source*: "Relative curvature measures of nonlinearity," by D. M. Bates and D. G. Watts, *Journal of the Royal Statistical Society*, **B-42**, 1980, 1–16, discussion 16–25.) Fit the nonlinear model

$$Y = \theta_1 X/(\theta_2 + X) + \epsilon$$

to the (simulated) data in the table by least squares, and provide a follow-up analysis of your results, including a plot of the data and fitted equation. Suppose you were asked to plan one more run. At what X-value would you take an observation Y? If you could plan *two* more runs instead, what would the best X-values be?

X	Y	X	Y
2.000	0.0615	0.286	0.0129
2.000	0.0527	0.286	0.0183
0.667	0.0334	0.222	0.0083
0.667	0.0258	0.222	0.0169
0.400	0.0138	0.200	0.0129
0.400	0.0258	0.200	0.0087

U. Refer to the model in Exercise T. A more general model of that type is

$$Y = (\theta_4 + \theta_1 X^{\theta_3})/(\theta_2 + X^{\theta_3}) + \epsilon.$$

Note that, when $\theta_4 = 0$, this model function passes through the origin; in such form it is called the Hill model. When $\theta_4 = 0$ and $\theta_3 = 1$, the so-called Michaelis–Menten form (shown in Exercise T) is reached. (See the paper "General model for nutritional responses of higher

organisms," by P. H. Morgan, L. P. Mercer, and N. W. Flodin, *Proceedings of the National Academy of Sciences, USA*, **72**, 1975, November, 4327–4331. For additional examples of the use of this model, see "New methods for comparing the biological efficiency of alternate nutrient sources," by L. P. Mercer, N. W. Flodin, and P. H. Morgan, *Journal of Nutrition*, **108**, 1978, August, 1244–1249.)

First fit the more general model to the data in Exercise T and then find "extra sum of squares" contributions for (1) θ_4 given θ_1, θ_2, θ_3; (2) θ_3 given θ_1, θ_2, assuming $\theta_4 = 0$; (3) θ_3, θ_4 given θ_1, θ_2. (Get these by difference of the two $S(\hat{\boldsymbol{\theta}})$ values for two models appropriately chosen, for each "extra SS.") Compare these "extra SS" values with the pure error mean square value s_e^2. What do you conclude? What model would you use to represent the data and why?

V. Fit the model (24.1.3) to each of the two sets of data below, and perform the standard analyses. What is the correlation between $\hat{\theta}_1$ and $\hat{\theta}_2$ in each case? How would you characterize these two data sets?

Data Set 1		Data Set 2	
t	Y	t	Y
0.2	0.142	1	0.445
0.4	0.240	2	0.585
0.6	0.329	3	0.601
0.8	0.381	4	0.532
1.0	0.455	5	0.470

W. You wish to fit the nonlinear model $Y = \theta_1\{1 - \exp(-\theta_2 t)\} + \epsilon$ to these data:

t	1	3	4	9
Y	0.47	1.17	1.42	2.19

The experimenter says: "I want you to use $\theta_{20} = 0.25$ as an initial estimate for θ_2. Please get me an initial estimate of θ_1?" What value θ_{10}, to one decimal place, would you suggest?

X. (*Source*: "Plant density and crop yield," by R. Mead, *Applied Statistics*, **19**, 1970, 64–81.) Fit the nonlinear model

$$\ln W_i = -\theta_1^{-1} \ln(\theta_2 + \theta_3 X_i^{\theta_4}) + \epsilon_i$$

to each set of data in the table. The variables are

W = mean yield per plant in grams,

X = planting density of an onion variety in plants per square foot.

Provide all the usual analyses and check the residuals. Can you suggest a simpler model that might fit pretty well?

Variety No. 1		Variety No. 2		Variety No. 3	
W	X	W	X	W	X
105.6	3.07	131.6	2.14	116.8	2.48
89.4	3.31	109.1	2.65	91.6	3.53
71.0	5.97	93.7	3.80	72.7	4.45
60.3	6.99	72.2	5.24	52.8	6.23
47.6	8.67	53.1	7.83	48.8	8.23
37.7	13.39	49.7	8.72	39.1	9.59
30.3	17.86	37.8	10.11	30.3	16.87
24.2	21.57	33.3	16.08	24.2	18.69
20.8	28.77	24.5	21.22	20.0	25.74
18.5	31.08	18.3	25.71	16.3	30.33

Y. (*Source*: "ROSFIT: An enzyme kinetics nonlinear regression curve fitting package for a microcomputer," by W. R. Greco, R. L. Priore, M. Sharma, and W. Korytnyk, *Computers and Biomedical Research,* **15**, 1982, 39–45. Copyright © 1982 Academic Press, Inc. Thanks go to William R. Greco, who supplied the data.) The data in the table come from an enzyme kinetics study described in the source article. Fit the "competitive inhibition" nonlinear model

$$Y = \theta_1 X_1 / \{\theta_2(1 + X_2/\theta_3) + X_1\} + \epsilon,$$

and provide the usual analyses. In particular, use the pure error to make an approximate test for lack of fit. (*Note*: Alternative models that were assessed as being poorer fits to the data are described in the source article.)

X_1	X_2	n_i	$Y_u \times 1000$
0.25	0	4	303, 310, 323, 310
0.5	0	4	451, 465, 479, 454
1.25	0	4	752, 694, 756, 723
2.5	0	3	950, 929, 964
3.75	0	4	1020, 1013, 1054, 1040
5.	0	3	1072, 1059, 1094
0.25	0.2	2	48, 48
0.5	0.2	2	88, 89
1.25	0.2	2	188, 177
2.5	0.2	2	318, 318
3.75	0.2	2	447, 447
5.	0.2	2	553, 545
0.25	0.5	2	21, 22
0.5	0.5	2	38, 36
1.25	0.5	2	81, 85
2.5	0.5	2	162, 150
3.75	0.5	2	225, 210
5.	0.5	2	294, 269
		$n = 46$	

Z. (*Source*: "On the use of mist nets for population studies of birds," by R. H. MacArthur and A. T. MacArthur, *Proceedings of the National Academy of Sciences, Washington, DC,* **71**, 1974, 3230–3233.) Mist nets are very fine thread nets used in bird-trapping studies. Birds so trapped are tagged and released after data are recorded on them. A study usually continues for a week or two at a chosen site. Suppose that:

N = number of birds in the local population,
p = the probability of a bird being trapped during the study,
t_u = time in days at which nets are checked, $u = 1, 2, \ldots, n$,
Y_u = number of birds caught for the first time at time t_u,
Q = number of drifting birds in the locality; these do not belong to the local population but may be trapped also.

In one such study, the following data were obtained:

t_u	0.5	1.5	2.5	3.5	4.5	5.5	6.5	7.5	8.5	9.5
Y_u	13	5	9	8	2	5	1	0	1	1

Fit by least squares to these data the models

(1) $Y_u = Q + pN \exp(-pt_u) + \epsilon_u$,
(2) As (1) but with $Q = 0$,

and thus obtain estimates of the parameters Q, p, and N. The usual nonlinear estimation analyses should also be provided. Comment on what you find. (For more on this topic, see also "The analysis of trapping records for birds trapped in mist nets," by B. F. J. Manly, *Biometrics*, **33**, 1977, 404–410; and "On a nonlinear regression problem in ornithology," by A. P. Gore and K. S. Madhava Rao, Technical Report No. 38, Department of Statistics, University of Poona, Pune—411 007, India.)

Table for Exercise 15Q, page 368

X_1	X_2	X_3	X_4	X_5	X_6	X_7	Y
1	0	0.33	7	2	1	1	36
1	0	0.75	2.3	1	2	1	33
1	0	0.45	1.7	1	3	1	33
1	1	0.52	1.7	1	3	1	33
1	1	0.52	3.6	1	2	1	35
1	1	1.25	1.7	1	2	1	36
2	0	2.67	7	1	1	2	40
2	0	0.83	2.3	1	1	2	38
2	0	2.00	7	1	1	1	43
2	0	2.25	1.7	1	1	1	36
2	0	1.50	1.7	2	1	1	37
2	1	0.38	3.6	1	1	1	41
2	1	0.25	1.7	1	1	2	40
1	0	0.47	1.7	1	4	1	36
1	0	0.88	7	1	1	1	39
2	0	0.40	1.7	1	4	1	38
2	0	1.73	7	1	4	1	43
2	0	0.58	1.7	1	1	2	38
2	0	0.75	3.6	1	1	2	38

Answer to 15Q.

Q. A model containing X_1 and X_4 explains $R^2 = 0.778$ of the variation, and the addition of other variables increases this but not by much. A two-way table of the observations arranged with respect to these two variables makes it clear that the trip home takes longer on all days and that Fridays should be avoided if possible.