2.4 THE METHOD OF LEAST SQUARES

Various criteria might be used to estimate the coefficients in a model from experimental data. For each of \( p \) data points, we can define the error \( e_j \) as the difference between the observation \( Y_j \), \( j = 1, 2, \ldots, p \), and the predicted model response \( y_j(x) \)

\[
Y_j - y_j = e_j \quad j = 1, \ldots, p
\]

The independent variables in the vector \( x \) can be different variables or different functions of the same variable, such as \( x, x^2, x^3 \), etc. The independent variables are assumed to be known exactly, or at least the error involved in each element of \( x \) is substantially less than that involved in \( Y \). You might think that the overall sum of the errors could be of utility as an objective function; however, this idea is not appropriate because such an objective function allows positive and negative errors to cancel. A second criterion would be to sum the absolute values of the errors

\[
f_1 = \sum_{j=1}^{p} |e_j| \tag{2.3}
\]

Another would be to minimize the absolute value of the maximum error. Both of these latter criteria can be used via library computer codes.

However, the classical error criterion is the quadratic error summation:

\[
f_2 = \sum_{j=1}^{p} e_j^2 \tag{2.4}
\]

Criterion \( f_2 \) is different from criterion \( f_1 \) in that it weights large errors much more than extremely small ones in estimating the coefficients. In addition \( f_2 \), when minimized, leads to an analytical solution for the unknown coefficients. In some cases, if the error in \( e_j \) is known or can be estimated, it is appropriate to use weighting factors for the \( e_j \) that are inversely proportional to the known error. By this procedure you reduce the confidence limits for the estimated dependent variable (Hald, 1952), but note that the confidence limits really are based on the degree of the experimental error as described in most texts on statistics. If weights are included in the summation, you would use

\[
f_3 = \sum_{j=1}^{p} w_j e_j^2 \tag{2.5}
\]

Let us use the linear model \( y = \beta_0 + \beta_1 x \) to illustrate the principal features of the least squares method to estimate the model coefficients with \( w_j = 1 \). The objective function is

\[
f_2 = \sum_{j=1}^{p} (Y_j - y_j)^2 = \sum_{j=1}^{p} (Y_j - \beta_0 - \beta_1 x_j)^2 \tag{2.6}
\]

There are two unknown coefficients, \( \beta_0 \) and \( \beta_1 \), and \( p \) known pairs of experimental values of \( Y_j \) and \( x_j \). We want to minimize \( f_2 \) with respect to \( \beta_0 \) and \( \beta_1 \). Recall from calculus that you take the first partial derivatives of \( f_2 \) and equate them to zero, to get the necessary conditions for a minimum (the rationale is described in more detail in Sec. 4.5)

\[
\frac{\partial f_2}{\partial \beta_0} = 0 = 2 \sum_{j=1}^{p} (Y_j - \beta_0 - \beta_1 x_j)(-1) \tag{2.7a}
\]

\[
\frac{\partial f_2}{\partial \beta_1} = 0 = 2 \sum_{j=1}^{p} (Y_j - \beta_0 - \beta_1 x_j)(-x_j) \tag{2.7b}
\]
Let $b_0$ and $b_1$ be the estimates of $\beta_0$ and $\beta_1$, respectively, obtained by solving Eqs. (2.7). (We use different symbols to distinguish between true values and estimated values.) Rearrangement yields a set of linear equations in two unknowns, $b_0$ and $b_1$

\[
\sum_{j=1}^{p} b_0 + \sum_{j=1}^{p} b_1 x_j = \sum_{j=1}^{p} Y_j
\]

\[
\sum_{j=1}^{p} b_0 x_j + \sum_{j=1}^{p} b_1 x_j^2 = \sum_{j=1}^{p} x_j Y_j
\]

The summation $\sum_{j=1}^{p} b_0$ is $(p)(b_0)$ and in the other summations the constants $b_0$ and $b_1$ can be removed from within the summation signs

\[
b_0(p) + b_1 \sum_{j=1}^{p} x_j = \sum_{j=1}^{p} Y_j \quad (2.8a)
\]

\[
b_0 \sum_{j=1}^{p} x_j + b_1 \sum_{j=1}^{p} x_j^2 = \sum_{j=1}^{p} x_j Y_j \quad (2.8b)
\]

The above two linear equations in two unknowns, $b_0$ and $b_1$, can be solved quite easily. The predicted value of $y$, $\hat{Y}$, is $\hat{Y} = b_0 + b_1 x$.

**EXAMPLE 2.2 APPLICATION OF LEAST SQUARES**

Fit the model $y = \beta_0 + \beta_1 x$ to the following data ($Y$ is the measured response and $x$ the independent variable)

<table>
<thead>
<tr>
<th>$x$</th>
<th>$Y$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>3</td>
<td>6</td>
</tr>
<tr>
<td>4</td>
<td>8</td>
</tr>
<tr>
<td>5</td>
<td>10</td>
</tr>
</tbody>
</table>

Solution. The computations needed to solve Eq. (2.8) are

$\sum x_j = 15 \quad \sum x_j Y_j = 110$

$\sum Y_j = 30 \quad \sum x_j^2 = 55$

Then

$6b_0 + 15b_1 = 30$

$15b_0 + 55b_1 = 110$

Solution of these two equations yields

$b_0 = 0 \quad b_1 = 2$

and the model becomes $\hat{Y} = 2x$ where $Y$ is the predicted value for a given $x$.

Now that we have presented the basic ideas of fitting a model using simple example, we will extend the procedure to a general model which is linear in the coefficients.

\[
y = \sum_{i=0}^{n} \beta_i x_i, \quad x_0 = 1 \quad (2.9)
\]

In Eq. (2.9) $x_0 = 1$, a constant, so that an intercept is included in the equation. There are $n$ independent variables $x_i$, $i = 1, \ldots, n$. Independent here means controllable, or adjustable, not functionally independent. Equation (2.9) is linear with respect to the $\beta_i$ but $x_i$ can be nonlinear. However, keep in mind that the values of $x_i$ will be substituted for $x_i$ prior to solving for the $\beta_i$, the estimates of $\beta_i$, hence the functional form of $x_i$ even if nonlinear is not a matter of concern. For example, if the model is quadratic
we specify
\[ x_0 = 1 \]
\[ x_1 = x \]
\[ x_2 = x^2 \]

and the general structure of Eq. (2.9) is satisfied.

Introduction of Eq. (2.9) into the objective function (2.4) gives

\[
f_2 = \sum_{j=0}^{p} (Y_j - y)^2
\]

\[
= \sum_{j=0}^{p} \left( Y_j - \sum_{i=0}^{n} \beta_i x_{ij} \right)^2
\]

The independent variables are now identified by a double subscript, the first index designating the independent variables \((i = 0, \ldots, n)\) and the second the sequence of \(p\) data points \((j = 1, \ldots, p)\).

Next, differentiate \(f_2\) with respect to \(\beta_0, \beta_1, \ldots, \beta_n\), and equate the \((n + 1)\) partial derivatives to zero, obtaining \((n + 1)\) equations in \((n + 1)\) unknown values of the estimated coefficients \((b_0, \ldots, b_n)\):

\[
b_0 \sum_{j=1}^{p} x_{0j}^2 + b_1 \sum_{j=1}^{p} x_{0j} x_{1j} + b_2 \sum_{j=1}^{p} x_{0j} x_{2j} + \cdots + b_n \sum_{j=1}^{p} x_{0j} x_{nj} = \sum_{j=1}^{p} Y_j x_{0j}
\]

\[
b_0 \sum_{j=1}^{p} x_{1j} x_{0j} + b_1 \sum_{j=1}^{p} (x_{1j})^2 + b_2 \sum_{j=1}^{p} x_{1j} x_{2j} + \cdots + b_n \sum_{j=1}^{p} x_{1j} x_{nj} = \sum_{j=1}^{p} Y_j x_{1j}
\]

\[
b_0 \sum_{j=1}^{p} x_{2j} x_{0j} + b_1 \sum_{j=1}^{p} x_{2j} x_{1j} + b_2 \sum_{j=1}^{p} (x_{2j})^2 + \cdots + b_n \sum_{j=1}^{p} x_{2j} x_{nj} = \sum_{j=1}^{p} Y_j x_{2j}
\]

\[
\vdots
\]

\[
b_0 \sum_{j=1}^{p} x_{nj} x_{0j} + b_1 \sum_{j=1}^{p} x_{nj} x_{1j} + b_2 \sum_{j=1}^{p} x_{nj} x_{2j} + \cdots + b_n \sum_{j=1}^{p} (x_{nj})^2 = \sum_{j=1}^{p} Y_j x_{nj}
\]

Note the symmetry of the summation terms in \(x_{ij}\). This set of \((n + 1)\) equations in \((n + 1)\) unknowns can be solved on a computer using one of the many readily available routines for solving simultaneous linear equations.

Equations (2.11) can be expressed in more compact form if matrix notation is employed (see App. B). Let

\[
b = \begin{bmatrix} b_0 \\ b_1 \\ \vdots \\ b_n \end{bmatrix}, \quad Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_p \end{bmatrix}, \quad X = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1n} \\ 1 & x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{p1} & x_{p2} & \cdots & x_{pn} \end{bmatrix}
\]

Equations (2.11) can then be expressed as

\[
X^T X b = X^T Y
\]

which has the formal solution via matrix algebra

\[
b = (X^T X)^{-1} X^T Y
\]