CURVE FITTING AND ANALYSIS OF VARIANCE

by Paul Peach

1. Introduction

One of the fundamental assumptions of science is that like causes produce like effects, and that if we know the causes and causal relationships involved, we can predict the effects. The discovery of causal relationships, and their description in mathematical form, are thus legitimate objects of scientific investigation.

The task is sometimes of formidable difficulty, and the difficulties are of two distinct types. First, there is the difficulty of determining what the causes are. Suppose for example that we wish to predict the weather in Washington, D.C., 24 hours hence. In a general way, we know that present temperature, wind direction, etc., are pertinent information. But it may well be that to predict weather for Washington we should do best to seek our data in some other place -- that is, we may need to know what is happening in Cleveland or Atlanta. It may also be that the most useful predictive information is unavailable, perhaps because we do not have a ship or a balloon at the right place and at the right time. The location of weather stations is determined by population or facilities, and existing stations are where they are, not because meteorologists believe that information from these special locations has unusual predictive value, but because at these locations there are cities, universities, airports, and so on. The task of deciding which data to use for prediction is thus complicated by the fact that we are mostly unsure what the best data are.

There appear to be problems in which the best predictions we can make are so poor that they are hardly better than random guesses. Perhaps the outstanding examples of phenomena that have so far defied prediction are found in economics. We need not assume that stock market movements and industrial depressions are exempt from the laws of cause and effect; but it certainly seems credible that economic laws involve so many predictors, and in such complicated ways, that their complete statement may be forever beyond our powers.

The second difficulty arises when we try to determine how the predictor quantities shall enter our prediction equation. Thus, the fuel consumption per mile of an automobile depends (among other things) upon the speed. But in order to predict the fuel consumption we might use any function of the speed -- the figure itself, its square or cube, its logarithm, or some other function. The task of constructing a prediction formula is quite similar to that of deciphering a cryptogram; there are to be sure some general principles we can follow, but success depends more on patience, imagination, experience, and possibly luck, than upon the systematic application of standard analytical techniques. It has the further complication that once a cryptogram has been deciphered we are seldom
left in any doubt of our success, whereas even when we have arrived at a valid prediction formula, we may still be unable to satisfy ourselves of its validity.

The first difficulty can be surmounted (if at all) through such knowledge of the phenomena under discussion as specialists in scientific fields are expected to have. The second difficulty is merely a challenge to the mathematical and scientific imagination of the researcher. There remain two jobs that are essentially statistical in character. The first of these is to determine numerical values for the constant coefficients that appear in every prediction equation. The second is to devise criteria for testing whether a proposed prediction formula is a "true" statement of natural law, or merely one of a set of empirical equations, any one of which might be equally capable of explaining our finite set of data.

We shall generally determine our coefficients by the method of least squares, which we shall study at some length in this monograph; this method is well known and the subject of a considerable literature. As for criteria of validity, there does not seem to be a systematic treatment in existence, and we shall have to essay a beginning.

2. Completeness

At best, no mathematical law can exactly predict even the simplest event; the number of predictors required for a really complete prediction equation is almost surely infinite. Discussion of this point hinges on the meaning we give to the word "complete". Words like complete, exact, true, perfect, express concepts only; in practice we do not expect quite to attain these ideals. Perhaps there is no such thing as a complete, true statement, in the sense that the statement covers all possible or conceivable cases and leaves unsaid nothing that is pertinent. Whether completeness in this sense would be useful is an academic question, since it seems we shall never attain it. Our attention will therefore be better devoted to the attainment of such an approach to completeness that the practical needs of some problem are satisfied. The acceptance of such compromises is commonplace in both science and everyday life, and gives rise to such popular phrases as "complete for all practical purposes". This is the only kind of "completeness" we shall talk about in the remainder of this monograph.

If we agree to accept something less than ultimate perfection as "completeness" it follows that any prediction made from such a "complete" statement of natural law will be subject to some error; this we shall call the error of prediction. Suppose now that the predicted event has happened, and we are making a measurement to see how close our prediction was. There will usually be a discrepancy between the observed and predicted measurements, but it would be a mistake to treat the whole discrepancy as an error of prediction. If we make several measurements on the same quantity, these measurements will themselves usually not agree, and the true value we are seeking to ascertain will remain somewhat doubtful due to these disagreements, which we shall call errors of ascertainment.

Errors of ascertainment are of two kinds. The first of these arises from the operation of measurement itself. To every measuring operation there attaches an error, the expected magnitude of which is usually known or knowable with considerable accuracy. We frequently assume that errors of measurement can be made as small as we please by taking many measurements and calculating an average; there is a fundamental theorem in statistics which states that the error of a mean can be made as small as we like provided we have enough independent samples from a stable population (we disregard exceptional cases such as that of the Cauchy distribution).
The second type of error may be called "error of identification". It arises from the circumstance that consecutive measurements supposedly of the same quantity are in fact of slightly different quantities, due to changes, either in the environment or in the thing being measured, which take place during the time required for the measuring operation. To illustrate, suppose we are measuring the height of a building by triangulation. We start with numbers obtained by direct observation — readings from tapes, protractors, thermometers, and the like, all subject to errors of measurement — and our final answer is calculated from these numbers and includes their errors, with perhaps errors of rounding added. If we repeat the operation and calculate an average we are betting on the tendency of errors to compensate each other, at least in part. Actually we soon reach a stage where further measurements do not add much to our information, because the building we are measuring does not, so to speak, stand still. It expands and contracts with heat and cold; it sways in the wind; its foundations settle gradually. These and other causes cast a shadow over the very meaning of what we are measuring. No amount of repeated measurement will remove this inherent instability; it can at best be delimited by definition (e.g., by reduction to standard conditions of temperature and pressure). That portion of the error of ascertainment which is due to the inherent instability of the thing measured (relative to its environment) we call the error of identification. We might write

\[
\text{Error of Ascertainment} = \text{Error of Measurement} + \text{Error of Identification};
\]

we can reduce errors of measurement in various ways (better instruments, skill, duplicate or replicate measurements) but the error of identification persists and imposes its uncertainty on every metric statement we can make.

We are now in a position to define "completeness" as we shall use the word from now on:

\[(2.01) \quad \text{A prediction formula is complete if its errors of prediction are of the same order of magnitude as the errors of ascertainment which attach to direct measurements.}\]

This means that when we can predict about as reliably as we can measure, we agree to regard our prediction formula as complete. Completeness thus becomes relative to a particular background or set of circumstances, and statements which are complete with respect to one background may be incomplete with respect to another. For instance, the statement "The planets move in elliptical orbits, with the sun at one of the foci" was complete when Kepler made it, but is so no longer, since we have better measurements today than Kepler had. It usually happens that when we open up a new field of science, statements formerly regarded as complete have to be extended or modified.

3. Degrees of Freedom

We must pause at this point to introduce the "degrees of freedom" concept, which has become basic to modern statistical inference. In order to develop this notion from fundamentals, let us begin with the simplest possible statistical problem, that of two independent observations of equal weight which contain the whole of the information available relative to the point at issue. We have been given these two measurements, and it is our task to summarize them in a meaningful way.

Let us call the measurements \(X_1\) and \(X_2\). In making our summary, we should
almost certainly begin by calculating the mean or average, represented by \( \bar{x} \). The formula is common knowledge:

\[
(3.01) \quad \bar{x} = \frac{1}{2}(x_1 + x_2).
\]

We note that this formula is a linear equation in \( x_1 \) and \( x_2 \), and that it defines a new number, \( \bar{x} \), as a linear function of \( x_1 \) and \( x_2 \).

Having calculated the mean, our next question might be "How well do the measurements agree?" To answer this we might calculate the difference:

\[
(3.02) \quad D = x_1 - x_2.
\]

Again we have a new number defined as a linear function of the observations.

What have we accomplished? We have transformed our original numbers \( x_1 \) and \( x_2 \) into two new numbers, \( \bar{x} \) and \( D \). The new numbers do not contain any new information, but they present the same information in, so to speak, a more informative way. Each of the new numbers, or statistics, presents a certain aspect of the entire original set, the first having the ordinary meaning of an average, the second affording some clue to the errors of ascertainment.

The point is important enough to justify some repetition. We start with observed numbers, or data, or observations; we transform these by means of linear equations, and end with calculated numbers, or statistics. The reason we go to this trouble is that each statistic concentrates within itself information relative to some particular aspect of the data. From equations (3.01) and (3.02) we can readily obtain \( \bar{x} \) and \( D \), given \( x_1 \) and \( x_2 \). The converse is also true, given \( \bar{x} \) and \( D \), we can calculate \( x_1 \) and \( x_2 \). Elementary algebra yields readily the equations

\[
(3.03) \quad \begin{align*}
\bar{x}_1 &= \bar{x} + \frac{1}{2}D, \\
\bar{x}_2 &= \bar{x} - \frac{1}{2}D.
\end{align*}
\]

The transformation is thus reversible. This means that the number pair \( (x_1, x_2) \) is exactly equivalent to the number pair \( (\bar{x}, D) \); given either pair, we can get the other. If one pair contains information relevant to some question, the other pair contains exactly the same information, neither more nor less.

It follows that we cannot construct a third statistic, call it \( Z_3 \), which will be anything more than a rehash of \( \bar{x} \) and \( D \). For suppose we define such a statistic by the equation

\[
Z_3 = ax_1 + bx_2,
\]

where \( a \) and \( b \) are any coefficients you please. Substituting from (3.03) we find that

\[
Z_3 = \bar{x}(a + b) + \frac{1}{2}D(a - b),
\]

which shows that any such statistic must be merely a composite of the two already calculated.

Summarizing the results so far obtained, we note that starting with two observations it is possible to obtain two derived numbers or statistics, and only two independent statistics. The set of derived numbers is logically and mathematically equivalent to the set of observed numbers, and we can obtain either set given the other. We may also note in passing that while our algebraic and arith-
metrical operations have transformed the data, there has been no increase in the amount of information. The principle is analogous to the conservation laws; thus, the carpenter who builds a chair does not increase the amount of wood, but merely presents the same wood in a more usable form. The mathematical principle involved here is the same as that which states that in order that a set of simultaneous linear equations may have a unique solution, we must have the number of equations and the number of unknowns equal.

One more step in the direction of generalization is necessary before we proceed. We have calculated the statistics $X$ and $D$, but so far as mathematics goes we might equally well have calculated any pair satisfying the equations

$$
Z_1 = a_1 X_1 + a_2 X_2 ,
$$
$$
Z_2 = b_1 X_1 + b_2 X_2 ,
$$
provided only that $a_1 b_2 \neq a_2 b_1$; if $a_1 b_2 - a_2 b_1 = 0$, our transformation will not be reversible. (Try it and see.)

Equations (3.04) give the most general kind of linear transformation; in fact, they are a bit too general for our present purpose. Special interest attaches to the class of transformations in which the following requirements are met:

$$
a_1 = a_2 ,
$$
$$
b_1 = -b_2 .
$$

A transformation which meets these requirements is said to be orthogonal. Orthogonal transformations are of special importance in statistics, since the transforms to which they lead have peculiarly valuable properties. In particular, if our data consist of random drawings from a normal population, the statistics derived by means of orthogonal linear transformations are independent in the probability sense; that is, they are uncorrelated.

Now let us extend our study to the next larger problem, in which we have three observations. These might be, for example, intelligence test scores on three people: call them Sam, Bob and Susie, with scores respectively $X_1$, $X_2$ and $X_3$. A little thought should make it clear that these observations can likewise be transformed into a set of derived numbers or statistics; that a complete set of statistics will contain exactly three of them; that such a set will be the mathematical and logical equivalent of the original data; and that it will not be possible to add a fourth statistic which will be anything more than a composite of the first three. One possible transformation is the following:

$$
Z_1 = X_1 + X_2 + X_3 ,
$$
$$
Z_2 = X_1 - X_2 ,
$$
$$
Z_3 = X_1 + X_2 - 2X_3 .
$$

Examining these, we see that $Z_1$ is equivalent to the mean, needing only to be divided by 3; $Z_2$ measures the difference between Sam and Bob; $Z_3$ measures the difference between the score of Susie and the mean score for the two men. It is easy to show that the $Z$'s are a complete set by solving the equations (3.06) for the $X$'s in terms of the $Z$'s.

When we have three equations, the orthogonality conditions are a bit more complicated; but they do not become more complicated when we go to four or more.
One way of stating them is as follows:

(3.07) 1. The coefficients of the X's for $Z_1$ are all equal.
2. The coefficients of the X's for each of the other Z's add to zero.
3. If for one of the Z's the coefficients of the X's are respectively $a_1, a_2, a_3$ and for another they are $b_1, b_2, b_3$, we must have

$$a_1b_1 + a_2b_2 + a_3b_3 = 0.$$  

It is easy to see that equations (3.06) satisfy the orthogonality conditions. However, (3.06) is not the only orthogonal set; in fact, there is an infinity of such sets, all having the same $Z_1$. To see this, let us write more generally

(3.08) $$Z_1 = X_1 + X_2 + X_3,$$
$$Z_2 = a_1X_1 + a_2X_2 + a_3X_3,$$
$$Z_3 = b_1X_1 + b_2X_2 + b_3X_3.$$  

From the orthogonality conditions of (3.07) we must have

$$a_1 + a_2 + a_3 = 0,$$
$$b_1 + b_2 + b_3 = 0,$$
$$a_1b_1 + a_2b_2 + a_3b_3 = 0.$$  

With a little algebra we are led to new equations from which $a_3, b_2$ and $b_3$ have been eliminated:

(3.09) $$Z_1 = X_1 + X_2 + X_3,$$
$$Z_2 = a_1X_1 + a_2X_2 - (a_1 + a_2)X_3,$$
$$Z_3 = b_1X_1 - \frac{b_1(2a_1 + a_2)}{a_1 + 2a_2} X_2 + \frac{b_1(a_1 - a_2)}{a_1 + 2a_2} X_3,$$

and in these equations the orthogonality conditions are satisfied no matter what values we give to $a_1, a_2$ and $b_1$.

To sum up: When we have three observations, or X's, we can if we like transform them into three new numbers or statistics, which we call Z's. One of these will generally be the arithmetic mean or its equivalent, which we shall designate by $Z_1$. The remaining two Z's may be defined in any convenient way, and even if we require that all the Z's be mutually orthogonal we still have the choice among an infinity of possibilities for these two Z's. We say we have two degrees of freedom.

Turning next to the problem of four observations, suppose that to our IQ's on Sam, Bob and Susie we add a fourth IQ, that of Gloria. In order to make the problem more definite, suppose the data are as follows:

$$\begin{align*}
\text{IQ of Sam} & \quad X_1 = 150, \\
\text{IQ of Bob} & \quad X_2 = 130, \\
\text{IQ of Susie} & \quad X_3 = 80, \\
\text{IQ of Gloria} & \quad X_4 = 60.
\end{align*}$$  

Among all the linear transformations we might make upon these data the following
one is of obvious interest:

\[ Z_1 = X_1 + X_2 + X_3 + X_4 \] (leading to the mean),
\[ Z_2 = X_1 - X_2 , \]
\[ Z_3 = X_3 - X_4 , \]
\[ Z_4 = X_1 + X_2 - X_3 - X_4 . \]

These \( Z \)'s have obvious meanings. \( Z_1 \) can be divided by 4 to give us the mean or average of the four scores. \( Z_2 = 20 \); this is the difference between the two men, and is relevant to the question "Are the two men equally intelligent?" \( Z_3 = 20 \) also, and does for the ladies what \( Z_2 \) does for the men. \( Z_4 = 70 \), and is relevant to the question "Is there any evidence of a difference due to sex?" (In order to make these differences comparable with each other they would need to be reduced to a common scale; we shall tackle this problem in due course.)

It is easy to show that our transformation is reversible, so that given the \( Z \)'s we can compute the \( X \)'s. Moreover, the equations of (3.10) are all mutually orthogonal, since for each pair of equations after the first we have

\[ a_1 + a_2 + a_3 + a_4 = 0 , \]
\[ b_1 + b_2 + b_3 + b_4 = 0 , \]
\[ a_1 b_1 + a_2 b_2 + a_3 b_3 + a_4 b_4 = 0 . \]

Save for the additional terms, these are the equations of (3.07).

Another orthogonal set, which would be useful for the interpretation of another series of measurements, is the following:

\[ Z_1 = X_1 + X_2 + X_3 + X_4 , \]
\[ Z_2 = X_1 - X_2 , \]
\[ Z_3 = X_1 + X_2 - 2X_3 , \]
\[ Z_4 = X_1 + X_2 + X_3 - 3X_4 . \]

Can you suggest a practical problem in which these would be meaningful?

* * *

Now to generalize: If we have a sample consisting of \( n \) observations suitable for statistical treatment, we may if we like calculate a set of derived numbers or statistics which will be logically and mathematically equivalent to the observations. The complete set will contain \( n \) statistics. One member of the set will usually be the mean. There will then remain \((n - 1)\) degrees of freedom for defining new statistics, which we may use in whatever way we please (though we shall generally prefer orthogonal transformations). Each degree of freedom may be regarded as leading to a definite statistic capable of measuring some specific effect or difference.

There is of course nothing in the rules of statistical procedure that requires us to convert every set of \( n \) measurements into a complete set of statistics, and
in point of fact this is hardly ever done. As a rule we are satisfied to calculate only the mean, and to use all the remaining degrees of freedom for estimating the variance or standard deviation. Nevertheless, there are many problems in which our purpose is best served by separating some of the degrees of freedom, as we shall see in due course.

4. The Method of Least Squares

Suppose we have some quantity \( y \) and related quantities \( z_1, z_2, \ldots \). We believe that some or all of the \( z \)'s can be used to predict \( y \); in fact, we may write

\[
(4.01) \quad y = f(z_1, z_2, \ldots) + e,
\]

where \( e \) is the error of prediction. Now let \( x_1, x_2, \ldots \), be some functions of the \( z \)'s which we have decided to use for prediction. Equation (4.01) can now be written

\[
(4.02) \quad y = \beta_1 x_1 + \beta_2 x_2 + \cdots + e,
\]

where the \( \beta \)'s are unknown constant coefficients. Our task is to estimate these coefficients, given a set of observations on \( y \) and the \( z \)'s. For this purpose we shall use the method of least squares.

We have as our raw material a set of measurements on \( y \) and the \( z \)'s. We assume that measurements on \( y \) are subject to errors of ascertainment, and we shall assume further that these errors are all independent of each other in a probability sense. For the purpose of elementary exposition we shall assume that each \( e \) is drawn at random from a stable population with finite variance; it is not usually necessary to assume that the mean of the errors is zero. (We shall see later that the requirement of uniform variance can be relaxed if we are willing to use weighting techniques.) For the present, we shall further assume that the \( z \)'s are subject to errors which can be disregarded by comparison with the errors of \( y \). It can then be shown that those estimates \( \hat{\beta}_1, \hat{\beta}_2, \ldots \) of the \( \beta \)'s are, in a sense, best, which make the sum of the \( e^2 \) as small as possible. We obtain an equation of the form

\[
(4.03) \quad Y = b_1 x_1 + b_2 x_2 + \cdots + b_p x_p
\]

such that the sum of all the differences \( (Y - y)^2 \) is a minimum.

The quantity

\[
(4.04) \quad Y - y = v
\]

is called a residual, \( Y \) being the value calculated from (4.03) and \( y \) the observed value. \( v \) is an estimate of the error \( e \), and what we actually minimize is the sum of the \( v^2 \) (which we shall write \( Sv^2 \)). Note that we think of three different kinds of values for the quantity under study:

1. The observed value, obtained by measurement, denoted by \( y \).
2. The calculated value, obtained from (4.03), denoted by \( Y \).
3. The true value, which remains unknown, denoted by \( \eta \) (eta).

The error is \( (\eta - y) = e \), but this is of course unknown, estimated by \( v \).
If we write

\[(4.05) \quad s^2 = [Y - y]^2 = (b_1 x_1 + b_2 x_2 + \ldots + b_p x_p - y)^2 \]

and differentiate with respect to each of the b's, then set each derivative equal to zero, we obtain

\[(4.06) \quad \begin{align*}
    b_1 s_{x_1}^2 + b_2 s_{x_1 x_2} + \ldots + b_p s_{x_1 x_p} &= s_{x_1 y}, \\
    b_1 s_{x_2}^2 + b_2 s_{x_2 x_2} + \ldots + b_p s_{x_2 x_p} &= s_{x_2 y}, \\
    &\vdots \\
    b_1 s_{x_p}^2 + b_2 s_{x_2 x_p} + \ldots + b_p s_{x_p x_p} &= s_{x_p y},
\end{align*}\]

which are called the normal equations of least squares. There are p equations in p unknowns, the unknowns being the b's. In general these equations will have a solution, which will give us those values of the b's which make \( s^2 \) a minimum.

The coefficients of the b's in the normal equations are the sums of squares and cross-products obtained from the data; thus, the coefficient of \( b_1 \) in the first equation is \( s_{x_1}^2 \), the sum of the squares of all the measurements on \( x_1 \). All this will be made clearer by working through a numerical example, and we introduce one without delay.

### 4.1. Numerical Example of Least Squares Problem

(The following example is selected for ease of computation; the data consist for the most part of small integers, and the operation of summing squares and cross-products can thus be followed with little difficulty. In least squares problems in general we may expect larger numbers and more of them; but for illustration our purpose is defeated if the arithmetical work casts an unnecessary shadow over the problem.)

When a job consists of a number of elementary operations and it becomes desirable to estimate the time required by each operation, direct measurement may be difficult or impossible. If we have the total time on various jobs that involve the same operations but in different numbers, we may be able to make a least squares estimate.

In the operation of electric computing machines many jobs consist of addition, multiplication, and copying down numbers. The following table shows, for ten different jobs, the number of operations of each kind, and also the total observed time (in seconds) required for the job's completion.

<table>
<thead>
<tr>
<th>Job No.</th>
<th>( x_1 )</th>
<th>( x_2 )</th>
<th>( x_3 )</th>
<th>( y )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>21</td>
<td>4</td>
<td>6</td>
<td>243.3</td>
</tr>
<tr>
<td>2</td>
<td>18</td>
<td>2</td>
<td>4</td>
<td>196.4</td>
</tr>
<tr>
<td>3</td>
<td>44</td>
<td>6</td>
<td>7</td>
<td>455.2</td>
</tr>
<tr>
<td>4</td>
<td>44</td>
<td>6</td>
<td>13</td>
<td>463.1</td>
</tr>
<tr>
<td>5</td>
<td>60</td>
<td>5</td>
<td>7</td>
<td>574.8</td>
</tr>
<tr>
<td>6</td>
<td>52</td>
<td>6</td>
<td>7</td>
<td>536.8</td>
</tr>
<tr>
<td>7</td>
<td>28</td>
<td>6</td>
<td>13</td>
<td>363.4</td>
</tr>
<tr>
<td>8</td>
<td>20</td>
<td>4</td>
<td>9</td>
<td>254.7</td>
</tr>
<tr>
<td>9</td>
<td>32</td>
<td>2</td>
<td>3</td>
<td>314.8</td>
</tr>
<tr>
<td>10</td>
<td>36</td>
<td>2</td>
<td>5</td>
<td>337.4</td>
</tr>
</tbody>
</table>
In Table 4.1.01, \( x_1 \) = number of addition operations,
\( x_2 \) = number of multiplication operations,
\( x_3 \) = number of copying operations,
\( y \) = time in seconds.

This table tells us, e.g., that Job No. 1 consisted of 21 additions, 4 multiplications, and 6 copying operations, and the reported total time was 243.3 seconds. We may feel some curiosity about how the interval was measured, and whether the time is really accurate to the tenth of a second; but these points do not bear directly upon the least squares solution. A more important question is whether it is reasonable to suppose that the expected error is the same for all jobs. One would suppose that the time required for a long job would be more variable than that required for a short one, and if we had more ample data we might investigate the question. In a short series we can hardly hope to draw any conclusion, and even if we had a set of weights we might well find that our answer was about the same as that found without weights. We turn from these brief considerations of the data to the least squares solution.

Our problem is to find an equation of the form

\[
(l.1.02) \quad b_1 x_1 + b_2 x_2 + b_3 x_3 = y
\]

which will enable us to estimate the total job time if we know how many operations of each kind the job involves — that is, if we know \( x_1 \), \( x_2 \) and \( x_3 \). Clearly \( b_1 \) will be the estimated time required for one addition, \( b_2 \) that required for one multiplication, and \( b_3 \) that required to copy a result. In order to write down the normal equations, we need the following sums of squares and cross-products:

\[
S_{x_1}^2 = (21)^2 + (18)^2 + (44)^2 + (44)^2 + \ldots + (36)^2 = 14,190.
\]
\[
S_{x_1 x_2} = (21)(4) + (18)(2) + (44)(6) + \ldots + (36)(2) = 1,626.
\]
\[
S_{x_1 x_3} = (21)(6) + (18)(4) + (44)(7) + \ldots + (36)(5) = 2,643.
\]
\[
S_{x_1 y} = (21)(243.3) + (18)(196.4) + \ldots + (36)(337.4) = 147,551.2
\]

and similarly we find \( S_{x_2}^2 = 213 \), \( S_{x_2 x_3} = 359 \), \( S_{x_2 y} = 17,474.2 \),
\[
S_{x_3}^2 = 652, S_{x_3 y} = 28,881.2, S_{y} = 1,547,855.2
\]

the last quantity, \( S_{y} \), does not appear in the normal equations, but we shall want it later. Our normal equations are as follows:

\[
(l.1.03) \quad 14,190 b_1 + 1626 b_2 + 2643 b_3 = 147,551.2,
\]
\[
1626 b_1 + 213 b_2 + 359 b_3 = 17,474.2,
\]
\[
2643 b_1 + 359 b_2 + 652 b_3 = 28,881.2
\]

and solving we find

\[
(l.1.04) \quad b_1 = 8.2368052094 \quad b_2 = 10.8001628928 \quad b_3 = 4.9602229340
\]

In practice we should of course report a smaller number of decimals, say two or three; the ten-decimal answers given here are to provide a basis of comparison.
between different computational methods which may give approximate answers. The answers of (4.1.04) were calculated by determinants and are exact as far as they go.

4.2. Numerical Solution of Normal Equations: Direct Method

In the solution of a set of simultaneous linear equations it is helpful to arrange the work in some definite order or tabular pattern. In the following table the solution of the equations (4.1.03) has been so arranged.

Table 4.2.01 Direct Solution of Normal Equations

<table>
<thead>
<tr>
<th>Line</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(14190 \cdot b_1 + 1626.0000 \cdot b_2 + 2643.0000 \cdot b_3 = 147551.20)</td>
</tr>
<tr>
<td>2</td>
<td>(1626 \cdot b_1 + 213.0000 \cdot b_2 + 359.0000 \cdot b_3 = 17474.20)</td>
</tr>
<tr>
<td>3</td>
<td>(2643 \cdot b_1 + 359.0000 \cdot b_2 + 652.0000 \cdot b_3 = 28881.20)</td>
</tr>
<tr>
<td>4</td>
<td>(b_1 + 0.1115877 \cdot b_2 + 0.1862579 \cdot b_3 = 10.398253)</td>
</tr>
<tr>
<td>5</td>
<td>(1626 \cdot b_1 + 186.3196 \cdot b_2 + 302.8553 \cdot b_3 = 16907.56)</td>
</tr>
<tr>
<td>6</td>
<td>(2643 \cdot b_1 + 302.8553 \cdot b_2 + 192.2796 \cdot b_3 = 27182.58)</td>
</tr>
<tr>
<td>7</td>
<td>(26.6804 \cdot b_2 + 56.1147 \cdot b_3 = 566.64)</td>
</tr>
<tr>
<td>8</td>
<td>(56.1147 \cdot b_2 + 159.7204 \cdot b_3 = 1398.62)</td>
</tr>
<tr>
<td>9</td>
<td>(b_2 + 2.10443425 \cdot b_3 = 21.2380624)</td>
</tr>
<tr>
<td>10</td>
<td>(56.1147 \cdot b_2 + 118.1147 \cdot b_3 = 1192.40)</td>
</tr>
<tr>
<td>11</td>
<td>(41.5127 \cdot b_3 = 206.20)</td>
</tr>
<tr>
<td>12</td>
<td>(b_3 = 4.96047)</td>
</tr>
</tbody>
</table>

The first three lines contain the equations to be solved. Line 4 is obtained from line 1 by dividing by the leading coefficient (that is, the coefficient of the first term, or 14190); the purpose is to make the coefficient of \(b_1\) equal to unity. Multiplying line 4 by the leading terms of lines 2 and 3 we obtain lines 5 and 6, and when these are subtracted from lines 2 and 3 we get lines 7 and 8, from which \(b_1\) has been eliminated. Line 9 is obtained from Line 7 by dividing by the leading term; line 10 by multiplying line 9 by the leading term of line 8; line 11 by subtracting line 10 from line 8. In line 12 we obtain a numerical value for the third unknown; the further solution for the other two should be obvious.

In this solution we have carried four decimal places most of the time, and our table has been constructed in such a way that we have uniform columns; this is desirable if we are to avail ourselves of the convenience of ruled paper and tabular forms for our solution. It has this drawback, that when we make the subtractions incident to eliminating the unknowns we may find our significant figures melting away. In the example, we started with seven figures on the right of the equality sign, but after the first elimination we find ourselves down to five. It is a good rule, in solving a set of normal equations, to carry as many decimals as the calculating machine is able to handle, so as to avoid the pyramiding of rounding errors in the course of the solution. After the solution has been obtained it is easy to drop as many of the superfluous decimals as one wishes.

We note incidentally that having carried a minimum of five significant figures throughout, our answer is not quite correct to five figures, but not bad.

The pencil-and-paper work of solving a set of equations can be further reduced by writing the solution in skeleton form, leaving out the b's and the plus and equals signs. We note further that many of the coefficients appear
twice; the normal equations are always symmetrical about the main diagonal, and we have chosen a method of solution that preserves this symmetry. In our skeleton form we shall show each coefficient only once, as this suffices for the solution.

Table 4.2.02 Skeleton Form for Direct Solution

<table>
<thead>
<tr>
<th>11190</th>
<th>1626.</th>
<th>2643.</th>
<th>117551.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>213.</td>
<td>359.</td>
<td>17174.2</td>
<td></td>
</tr>
<tr>
<td>652.</td>
<td></td>
<td>28881.2</td>
<td></td>
</tr>
<tr>
<td>11587</td>
<td>.1862579</td>
<td>10.3982523</td>
<td></td>
</tr>
<tr>
<td>186.3196</td>
<td>302.8553</td>
<td>16907.56</td>
<td></td>
</tr>
<tr>
<td>492.2796</td>
<td>27482.58</td>
<td></td>
<td></td>
</tr>
<tr>
<td>26.6804</td>
<td>56.1447</td>
<td>566.64</td>
<td></td>
</tr>
<tr>
<td>159.7204</td>
<td>1398.62</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.1043425</td>
<td>21.2380624</td>
<td></td>
<td></td>
</tr>
<tr>
<td>56.1447</td>
<td>118.1477</td>
<td>1192.40</td>
<td></td>
</tr>
<tr>
<td>115.5727</td>
<td>206.28</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4.96017</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The arithmetical work is as before. Entries omitted because of symmetry are simply ignored.

The direct method has the advantage that it can be followed by anyone who remembers high school algebra, but it is not the most efficient computationally. A more efficient method was devised by M. H. Doolittle of the U. S. Coast and Geodetic Survey, and published in 1878. This method, modified to take advantage of the capabilities of modern calculating machines, will be most efficient for a large number of problems and highly efficient for others. It is known as the Abbreviated Doolittle Method, and we shall represent it by the letters ADM.

4.3. The Abbreviated Doolittle Method

The success of the Abbreviated Doolittle Method depends upon the fact that modern calculating machines such as the Monroe, the Marchant, and the Friden, can accumulate sums and differences of products. Thus, in obtaining e. g. \( Sx_1x_2 \) for our normal equations, it is not necessary to write down each of the \( n \) products and then add them; we can perform the multiplications one after the other and allow the products to accumulate in the machine, merely copying the total at the end. (It is necessary, of course, always to use the same placing of decimal points in the multiplicand and multiplier.) Most of our arithmetic in solving the normal equations can be reduced to operations of the type

\[
ab - cd \quad \text{or} \quad (ab - cd)/k,
\]

and in either case we can go directly to the answer without copying down any of the intermediate results.

The student may find it interesting to prove that the algorithm we are about to present is in reality exactly equivalent to the direct method. Part of the equivalence should be obvious, as many of the numerical entries are identical.
In skeleton form, we have for the ADM:

<table>
<thead>
<tr>
<th>Line</th>
<th>14190</th>
<th>1626.</th>
<th>2643.</th>
<th>14751.2</th>
<th>166010.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>213.</td>
<td>359.</td>
<td>17471.2</td>
<td>19672.2</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>652.</td>
<td>28881.2</td>
<td>32535.2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>1115977</td>
<td>1862579</td>
<td>10.3982523</td>
<td>11.6990980</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>26.68040</td>
<td>56.1145877</td>
<td>10.3982523</td>
<td>11.6990980</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>4.9602b</td>
<td>4.9602b</td>
<td>4.9602b</td>
<td>4.9602b</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The asterisks *** indicate entries which must be calculated but need not be written down. Line 5 is calculated to 7 decimals in order that Line 6 may have seven significant figures, which means five decimals. The method of calculating the entries in each line is as follows:

Lines 1, 2 and 3 are as in Table 4.2.02; they contain the problem to be solved. There is one difference: an extra column has been added at the end. This is a check column, and should always be carried as a matter of routine, since by its means errors can usually be discovered promptly. (The student who needs convincing should do a few examples without a check column and then go back and try to find errors.) Each entry in the check column is equal to the sum of all the other entries in the same line, including those which have been omitted on account of symmetry or for other reasons. Thus, to obtain the check entry for Line 2 we must include in the total 1626, which would appear in the first space but has been omitted because of symmetry. In Line 3 we must supply 2643 and 359. The easiest way to do this is to sum along an L-shaped path; thus, for the second line we start at the head of the second column, turn the corner at the diagonal entry 213, and so to the end. For Line 3 we start at the head of the third column, go down to the third line, then turn the corner. The totals for Lines 5, 7 and 9 must be increased by unity, which would be the first entry in those lines but can be omitted as it is not needed for the calculations. The check column is treated like the other columns; we get the entries first by the ADM algorithm, then sum the entries in the line; if the two figures check we assume there is no error in that line.

Line 4 is exactly the same as Line 1, and is obtained by mere copying. Line 5 is obtained from Line 4 by dividing each entry by the leading term = 14190. The entry in the check column is obtained in the same way; 166010.2/14190 = 11.6990980. The sum of the entries on Line 5 is 11.6990979, which is a satisfactory check. (We must be prepared for small differences in the last decimal place.) In arriving at the sum we must supply the 1 which would appear under the leading term, but has not been written down.

The forward part of the ADM solution consists of pairs of lines, always related in the same way: the second line is obtained from the first by dividing each entry by the leading term. It is thus convenient to draw lines between the pairs, and incidentally this facilitates the solution itself, as we shall see.

We now compute Line 6. The entries in this line are obtained from the corresponding entries of Line 2. From each of these we subtract the product of two entries, one taken from Line 4 and the other from Line 5. The procedure is best
indicated, perhaps, by displaying the actual arithmetical operations.

For the first entry in Line 6 we begin with the first entry in Line 2, which is 213. Reading down the column we find the numbers 1626 and .1145877; these are the factors whose product is to be subtracted from 213. We set up 213 in the machine, allowing enough decimals for the product; then reverse-multiply .1145877 by 1626 and read the remainder = 26.68040 in the dial. On Monroe and Friden machines the operation is as simple as direct multiplication; the Marchant is less easy to use, as the "reverse" key must be kept pressed down by hand. The arithmetic is indicated by the equation

\[ 213 - (1626)(.1145877) = 26.68040. \]

The second entry in Line 6, and the one immediately beneath it in Line 7, may be calculated in succession. We start with the second entry in Line 2, which is 359. From this we subtract the product of a pair of numbers from Lines 4 and 5; we may take either

\[ 359 - (1626)(.1862579) = 56.1465 \]

or

\[ 359 - (2643)(.1145877) = 56.1465. \]

this element of choice characterizes AIM. The rule is: One factor from the same column as the number we start with, the other from the "leading column" -- that is, the column that contains the first entry for the line we are reducing. We are at present working on Line 2, whose first entry appears in Column 2; thus, Column 2 is now the leading column and one of our factors is taken from it. The number we are reducing is 359, which appears in the third column; so we take the other factor from the third column. We may call the products (1626)(.1862579) and (2643)(.1145877) diagonal products, since they indicate the diagonals of a rectangle whose boundaries are Line 4, Line 5, Column 2 and Column 3.

In taking out diagonal products, the question naturally arises: Which of the two possible pairs of factors should we use? The rule is: Use the pair whose elements are most nearly equal. In the present example we should prefer (1626)(.1862579) to (2643)(.1145877). The purpose of this rule is to minimize rounding errors, to which our decimal numbers will in general be subject. Since for convenience we shall usually stick to a fixed number of decimal places throughout our solution, it follows that on the average the rounding error will be proportionately largest for the smallest number; our rule tells us to avoid using this as one of the factors.

As soon as we have obtained the second entry in Line 6 we divide it by the first, obtaining

\[ 56.1465/26.68040 = 2.10434; \]

the corresponding entry in Line 7. It is of course possible to calculate Line 6 clear through, then go back and divide each entry by 26.68040 to get Line 7; but this method involves clearing the product out of the machine, then putting it back in again later, thus increasing the labor, creating a new possibility for mistakes, and introducing a new rounding error.

The last two entries of Line 6 must be calculated, but they are at once divided by the leading term and need not be written down. As before, we begin with a number in Line 2 and take out a diagonal product from lines 4 and 5, one factor coming from the leading column (in this case, Column 2), the other from the column which contains the number we originally put into the machine. We
obtain \[ 17474.2 - (1626)(10.3962523) = 566.64176 \]

but this number is not needed for our solution, so we divide it at once by 26.68040 to obtain 21.23813, which is written down in Line 7. For the last column we have

\[ 19672.2 - (1626)(11.6990980) = 649.46665 \]

\[ 649.46665/26.68040 = 24.34247 \]

which checks our arithmetic, the sum of the other entries in the line being equal to 24.34246. (Note that if we try to check Line 6 we don't do so well, since our check entry has eight figures and we are only carrying seven.)

We turn next to Line 8 and begin by setting up in the machine the first number from Line 3 (= 652). Beneath it in the same column are two pairs of numbers, one in the 4-5 section and one in the 6-7 section (i.e., lines 6 and 7). We take out both the indicated products, thus:

\[ 652 - (2643)(1.1862579) - (56.14465)(2.10434) = 41.57294 \]

This is the only entry in Line 8 that needs to be written down. For the last two columns we have

\[ 28881.2 - (2643)(10.3982523) - (56.14465)(21.23613) = 206.21180 \]

and this number is immediately divided by the leading term:

\[ 206.21180/41.57294 = 4.96024 \]

which we enter in Line 9.

For the check column we have

\[ 32535.2 - (2643)(11.6990980) - (56.14465)(24.34246) = 247.78509 \]

\[ 247.78509/41.57294 = 5.96025, \text{ which checks.} \]

The rest of the unknowns can be obtained without writing down any more figures except the answers. In order to make the principle evident, let us examine Lines 7 and 9. In skeleton form they represent the equations

\[ b_2 + 2.10434 b_3 = 21.23813 \]

\[ b_3 = 4.96024 \]

To get \( b_2 \) we should clearly calculate

\[ b_2 = 21.23813 - 2.10434 b_3 \]

\[ = 21.23813 - (2.10434)(4.96024), \]

a simple operation which we can perform in the machine without writing down any new numbers. The answer is 10.80010.

So also for obtaining \( b_1 \) we note that Line 5 expresses in skeleton form

\[ b_1 + .1145877 b_2 + .1862579 b_3 = 10.3982523, \]
whence

\[ b_1 = 10.398253 - (1.1145877)(10.80010) - (0.1862579)(4.96024) = 8.23681. \]

The check column should be carried along to the end; we have for the last two entries

\[
\begin{align*}
24.34246 - (2.10434)(5.96025) &= 11.80007 \\
11.699080 - (1.1145877)(11.80007) - (0.1862579)(5.96025) &= 9.23681,
\end{align*}
\]

checking the final answers. (Remember that the figure in the check column includes the coefficient unity, omitted from the written entries.)

In order to present the ADM in a more general way, we include a problem in which the entries are indicated merely by symbols, and the operations by equations. The problem presented is what is called a five-by-five matrix; that is, five equations in five unknowns.

### 4.4 Symbolic Presentation of the Abbreviated Doolittle Method

In the symbolic presentation of ADM we divide the written work into three main parts. The first part consists of \( n \) lines and \((n + 2)\) columns, the last being the check column. This part contains the statement of the problem in skeleton form; the first line represents the first normal equation, and so on. The first line will contain \((n + 2)\) entries, the second \((n + 1)\), and so on, diminishing by unity at each step, until we reach the \( n \)th line, which always contains exactly three entries.

Each entry in the first part is represented by the letter \( a, g \) or \( j \). The \( j \) entries are those in the check column, and \( j_6 \) means the \( j \)-entry for the \( 6 \)th line. The \( g \) entries are those of the last column but one. Looking back at (4.06) we note that on the right side of the normal equations we have always quantities of the form \( Sx_iy \); these are our \( g \)'s. We have

\[
\begin{align*}
(4.4.01) &\quad g_1 = Sx_1y \quad g_2 = Sx_2y \quad g_3 = Sx_3y \quad \text{and so on.}
\end{align*}
\]

Still looking at (4.06) we see that all the coefficients on the left are of the form \( Sx_i \) (which becomes \( Sx_i^2 \) when \( i = j \)). For these we substitute the simpler form \( \hat{a}_{i,j} \). We have thus

\[
\begin{align*}
(4.4.02) &\quad a_{11} = Sx_1^2 \quad a_{22} = Sx_2^2 \quad a_{12} = Sx_1x_2 \quad \text{and so on.}
\end{align*}
\]

After the first part, or statement of the problem, we have the second part, which is called the forward solution. This part consists of a number of sections, of which each save the last consists of two lines, an \( A \) line and a \( B \) line. The \( A \) line is calculated from entries above it in the solution; the \( B \) line is obtained from the \( A \) line by dividing each entry of the \( A \) line by its leading term. (The first \( B \) is always equal to unity and need not be written down.) The check column is carried along as before; asterisks show values which must be calculated but need not be copied.

The third part contains the back solution, in which we obtain the answers to our problem. There are two entries in each line, the second or check entry being always one unit larger than the first or solution entry.
The first \( n \) rows contain the statement of the problem, i.e., the coefficients of the normal equations.

Forward solution begins here:

<table>
<thead>
<tr>
<th>( a_{11} )</th>
<th>( a_{12} )</th>
<th>( a_{13} )</th>
<th>( a_{14} )</th>
<th>( a_{15} )</th>
<th>( g_1 )</th>
<th>( j_1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a_{22} )</td>
<td>( a_{23} )</td>
<td>( a_{24} )</td>
<td>( a_{25} )</td>
<td>( g_2 )</td>
<td>( j_2 )</td>
<td></td>
</tr>
<tr>
<td>( a_{33} )</td>
<td>( a_{34} )</td>
<td>( a_{35} )</td>
<td>( g_3 )</td>
<td>( j_3 )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( a_{44} )</td>
<td>( a_{45} )</td>
<td>( g_4 )</td>
<td>( j_4 )</td>
<td>( g_5 )</td>
<td>( j_5 )</td>
<td></td>
</tr>
</tbody>
</table>

Forward solution ends here:

<table>
<thead>
<tr>
<th>( A_{11} )</th>
<th>( A_{12} )</th>
<th>( A_{13} )</th>
<th>( A_{14} )</th>
<th>( A_{15} )</th>
<th>( A_{16} )</th>
<th>( j_6 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( B_{12} )</td>
<td>( B_{13} )</td>
<td>( B_{14} )</td>
<td>( B_{15} )</td>
<td>( B_{16} )</td>
<td>( j_7 )</td>
<td></td>
</tr>
<tr>
<td>( A_{22} )</td>
<td>( A_{23} )</td>
<td>( A_{24} )</td>
<td>( A_{25} )</td>
<td>( g_6 )</td>
<td>( j_8 )</td>
<td></td>
</tr>
<tr>
<td>( B_{23} )</td>
<td>( B_{24} )</td>
<td>( B_{25} )</td>
<td>( B_{26} )</td>
<td>( j_9 )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( A_{33} )</td>
<td>( A_{34} )</td>
<td>( A_{35} )</td>
<td>( g_7 )</td>
<td>( j_{10} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( B_{34} )</td>
<td>( B_{35} )</td>
<td>( B_{36} )</td>
<td>( j_{11} )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( A_{44} )</td>
<td>( A_{45} )</td>
<td>( g_8 )</td>
<td>( j_{12} )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( B_{45} )</td>
<td>( B_{46} )</td>
<td>( j_{13} )</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( A_{55} )</td>
<td>( g_9 )</td>
<td>( j_{14} )</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Solution completed.

It is of course permissible to substitute the values of the \( b \)'s in the normal equations to see whether they check; but such a check is not very sensitive. If the check column has been carried to the end the chance of error is not great.

Equations for the entries in the above table are:

\[
\begin{align*}
    j_1 &= a_{11} + a_{12} + a_{13} + a_{14} + a_{15} + g_1 \\
    j_2 &= a_{12} + a_{22} + a_{23} + a_{24} + a_{25} + g_2 \\
    j_3 &= a_{13} + a_{23} + a_{33} + a_{34} + a_{35} + g_3 \\
    j_4 &= a_{14} + a_{24} + a_{34} + a_{44} + a_{45} + g_4 \\
    j_5 &= a_{15} + a_{25} + a_{35} + a_{45} + a_{55} + g_5.
\end{align*}
\]
The first row of the forward solution is the same as the first row of the statement of the problem, that is,

\[ A_{11} = a_{11} \quad A_{12} = a_{12} \quad \ldots \quad A_{16} = g_1 \quad j_6 = j_1. \]

The row of B's is obtained by dividing each A by A_{11}:

\[ B_{12} = A_{12}/A_{11} \quad B_{13} = A_{13}/A_{11} \quad \ldots \quad B_{16} = A_{16}/A_{11} \quad j_7 = j_6/A_{11}. \]

At this point we check; we should have

\[ B_{12} + B_{13} + B_{14} + B_{15} + B_{16} + 1 = j_7; \]

the extra 1 is added because B_{11} = 1, though it need not be written down.

For Line 8 we have first

\[ A_{22} = a_{22} - A_{12}B_{12}, \text{ then } \]

\[ A_{23} = a_{23} - A_{12}B_{13}, \quad \text{ or } \quad A_{23} = a_{23} - A_{13}B_{12}. \]

We have already noted that the diagonal products A_{12}B_{13} and A_{13}B_{12} are equal save for rounding errors, and stated the rule that those factors which are most nearly equal should be preferred. For brevity, in the remaining equations only one of the possible choices of pairs of factors will be indicated.

As soon as we have A_{23}, before clearing it out of the machine, we should at once divide to get B_{23}:

\[ B_{23} = A_{23}/A_{22}. \]

Next,

\[ A_{24} = a_{24} - A_{12}B_{14}, \quad B_{24} = A_{24}/A_{22} \]

\[ A_{25} = a_{25} - A_{12}B_{15}, \quad B_{25} = A_{25}/A_{22} \]

\[ A_{26} = g_2 - A_{12}B_{16}, \quad B_{26} = A_{26}/A_{22} \]

We have to compute A_{26} to get B_{26}, but A_{26} is not copied; so also with j_8:

\[ j_8 = j_2 - A_{12}j_7, \quad j_9 = j_8/A_{22}. \]

We now perform our check addition, and should have very nearly

\[ B_{23} + B_{24} + B_{25} + B_{26} + 1 = j_7. \]

The 10th row involves subtracting two diagonal products:

\[ A_{33} = a_{33} - A_{13}B_{13} - A_{23}B_{23} \]

\[ A_{34} = a_{34} - A_{13}B_{14} - A_{23}B_{24} \]

\[ A_{35} = a_{35} - A_{13}B_{15} - A_{23}B_{25} \]

\[ A_{36} = g_3 - A_{13}B_{16} - A_{23}B_{26} \]

\[ j_{10} = j_3 - A_{13}j_7 - A_{23}j_9 \]

As before, A_{36} and j_{10} need not be written down. The check summation is
Curve Fitting and Analysis of Variance

\[ B_{34} + B_{35} + B_{36} + 1 = j_{11} \]

The 12th row involves subtracting three diagonal products:

\[
P_{44} = a_{44} - A_{14}B_{14} - A_{24}B_{24} - A_{34}B_{34} \\
P_{45} = a_{45} - A_{15}B_{15} - A_{25}B_{25} - A_{35}B_{35} \\
P_{46} = a_{46} - A_{16}B_{16} - A_{26}B_{26} - A_{36}B_{36}
\]

For a check we should have:

\[ B_{45} + B_{46} + 1 = j_{13} \]

Concluding the forward solution, we have:

\[ A_{55} = a_{55} - A_{15}B_{15} - A_{25}B_{25} - A_{35}B_{35} - A_{45}B_{45} \]

\[ A_{56} = a_{56} - A_{16}B_{16} - A_{26}B_{26} - A_{36}B_{36} - A_{46}B_{46} \]

and then immediately, without clearing the machine:

\[ b_5 = A_{56}/A_{55} \]

Now the check column:

\[ j_{14} = j_5 - A_{15}j_7 - A_{25}j_9 - A_{35}j_{11} - A_{45}j_{13} \]

\[ b_5 + 1 = j_{15} \]

The remainder of the work, or "back solution", is shown by the equations:

\[ b_4 = B_{46} - B_{45}b_5 \]

\[ j_{16} = j_{13} - B_{45}j_{15} \]

\[ b_3 = B_{36} - B_{35}b_5 - B_{34}b_4 \]

\[ j_{17} = j_{11} - B_{35}j_{15} - B_{34}j_{16} \]

\[ b_2 = B_{26} - B_{25}b_5 - B_{24}b_4 - B_{23}b_3 \]

\[ j_{18} = j_9 - B_{25}j_{15} - B_{24}j_{16} - B_{23}j_{17} \]

\[ b_1 = B_{16} - B_{15}b_5 - B_{14}b_4 - B_{13}b_3 - B_{12}b_2 \]

\[ j_{19} = j_7 - B_{15}j_{15} - B_{14}j_{16} - B_{13}j_{17} - B_{12}j_{18} \]

Each of the last five \( j \)'s should exceed the corresponding \( b \) by unity for the check.

Minor variations of one kind or another can be introduced. Some computers, in going from the A's to the B's, change the signs of the B's, each \( B_{ii} \) becoming \(-1\). There is no harm in this, though there seems little point to it either. If the signs of the B's are changed, then all the minus signs in the above equations become plus. The difference in the resulting solution will be in notation only; the operations in the machine will be identical. The notation we have adopted has
been chosen for ease of understanding; mathematicians interested in studying the method algebraically will probably prefer the notation used by Dr. Paul Dwyer in his article "The Solution of Simultaneous Equations" (Psychometrika, Vol. 6, pp. 101-129, April 1941; see pages 110-112 for the ADM).

Note: The paper just cited, by Dwyer, gives a number of methods for the solution of simultaneous equations and the inversion of matrices. Of these, the present writer prefers ADM. In the same paper Dwyer describes a method, original with him, which he calls the Compact Method. In a later paper ("The Square Root Method and Its Use in Correlation and Regression", Jour. Amer. Stat. Assn., Vol. 40, pp. 493-503, Dec. 1945) Dwyer describes another original method, closely related to ADM but more compact — as compact, indeed, as the Compact Method. The square root method was adopted by D. B. Duncan and J. E. Kenney for their monograph "On the Solution of Normal Equations and Related Topics" (Edwards Bros., Ann Arbor, Mich., 1946).

In both the Compact and the Square Root methods the double rows of ADM are replaced by single rows. There is thus a saving in copying time, about what we might get by omitting the A rows of ADM. The computational work for the forward solution is approximately equal for all three methods. In the back solution, a final division is required for each b in the Compact and Square Root methods; this division is avoided by ADM because each $A_{ij} = 1$. Since for ADM we obtain the first b by division, the net difference amounts to $(n - 1)$ extra divisions for the Compact and Square Root methods; ADM avoids these divisions at the cost of carrying n extra rows in the forward solution.

For the solution of a set of simultaneous equations the Square Root and Compact methods appear to be somewhat more efficient than ADM, though for most of the problems likely to be encountered the advantage will be very small. In fitting a straight line the Square Root method uses 16 tabular entries, and ADM uses 19; two of these are $A_{13}$ and $A_{23}$, which can be omitted if desired. For three equations in three unknowns the Square Root method uses 28 entries, ADM 33, of which again two can be eliminated. Even the slightest numerical complication will wipe out the advantage obtained by using the Square Root Method.

Nevertheless, if all problems in least squares were simply the solution of a set of normal equations, the Square Root and Compact methods would be worth including in a monograph of this kind. As we shall soon see, most problems in least squares involving anything more complicated than a straight line are best handled through the inverse matrix. The inverse matrix can be calculated by any of the methods mentioned, but ADM is definitely the most efficient for this purpose; the loss through making extra entries is more than offset by the gain in computational labor.

To sum up: While there are certainly problems for which the Compact and Square Root methods are more efficient than ADM, yet at best the advantage is usually small. It looks greater than it really is because there are fewer tabular entries for the Compact and Square Root methods; we should remember that copying down entries is the least laborious part of the work. ADM at its worst is highly efficient, and at its best is by far the most efficient method yet proposed. For this reason, no description of the alternative methods is included here. Students who are interested can go to the publications cited.

A method proposed in 1941 by Dr. P. D. Crout is similar in principle to ADM, though superficially different. It is available from Marchant Calculating Machine Co., Oakland, Calif., as MM-182, Mathematics, Sept. 1941.
5. Computation of Sums of Squares and Cross Products

Before the introduction of modern calculating machines the computation of sums of squares and cross-products was regarded as the most laborious part of most least squares problems. Today even the biggest set of data can be worked up easily by using punch card methods, and smaller sets without undue labor on electric desk computers. We shall describe three methods, each with a definite scope.

5.01 Direct Multiplication Method

The direct multiplication method has already been mentioned; it consists of making the multiplications in succession and allowing the products to accumulate in the machine. It is a universal method, always applicable regardless of the type of data. It can be used with all models of Monroe, Marchant and Friden machines, but works most easily with the Friden and Monroe models equipped for automatic multiplication. The Marchant is clumsy to use when some of the products are negative. Monroe machines equipped with automatic squaring are especially convenient for this job.

Note: A word of comparison may be in place here concerning the three electric desk calculators, the Monroe, Marchant and Friden. Each of these machines is available in several models; our comparison will be based on the most versatile (and most expensive) stock model of each.

The Marchant is a rugged machine, with a good reputation for not getting out of order easily. For straight multiplication it is faster than either of the other machines. It has a "Reverse" key for negative multiplication, which releases itself after each digit of the multiplier; it is thus impossible to leave it down absent-mindedly, but on the other hand it has to be depressed for each digit in the multiplier, or else held down by hand while the multiplication is being made; most operators find this a nuisance, and in fact the Marchant is not recommended when there is a mixture of plus and minus products. Used as an adding machine, the Marchant has no "Repeat" key. This makes it impossible to use the method for extracting square root which can be carried out readily on the other machines. For division and subtraction all the machines are about equal. Taking all these points into consideration, the Marchant is probably the least well adapted to the calculations involved in curve fitting and correlation of all the common machines.

The Friden has the drawback that even on the most expensive model it is possible to get wrong answers. In least squares work it is frequently advisable to carry seven decimals in each factor, which of course means 14 for the product. If we compute the value of

\[ 7.0000000 - (1.2214102)(.1691426) = 6.0605614 \]

on the Friden we get the answer 7.0605614. The machine rings a bell when this sort of thing happens, but while the bell tells us that we have a wrong answer, it does not supply us with the right one. The difficulty can be surmounted in various ways, provided the bell does not get out of order. The Friden has the heaviest touch of all the machines. For sums of squares and cross products the Friden is less convenient than the Monroe but more so than the Marchant, since plus and minus factors are handled with equal ease. For general statistical work the Friden is very flexible and in particular the Abbreviated Doolittle Method is carried out as easily on the Friden as on any machine. The Friden has the reputation of being sturdy.

Until recently the best Monroe machine was the AA-1 model with automatic multiplication and a squaring lock for automatic sums of squares. In point
of convenience, this machine leaves little to be desired. It is fast, readily adapted to most statistical computations, and has the lightest touch of all the machines. But it has a bad reputation for getting out of order, not too serious a fault if stand-by machines and good repair service are available, but still unwelcome. There is now available a new model called to Monroe-Matic, which is quite different in design, does the same jobs as the AA-1, and is supposed to be much sturdier. If this latter promise is kept, the Monroe-Matic should become the statistical machine par excellence.

Mention should be made here of the Monroe LA-5 and similar models. These are small, portable machines, driven by an electric motor but hand operated. They can be had with or without automatic division. They are much cheaper than the automatic models, and exceptionally rugged, seldom needing repair. With a little skill, a computer can work nearly as fast on one of these as on a fully automatic machine. They are especially useful where the same machine must be used by many different people, not all skillful.

* * *

In figuring sums of cross products, say $5X_1X_2$, by the direct method, we may carry out the computation using $X_1$ as the multiplier and $X_2$ as the multiplicand. At the conclusion we shall have $5X_1X_2$ in one dial and $SX_1$ in the other. We may now repeat, but using $X_2$ as multiplier and $X_1$ as multiplicand. The sum of products should be the same, and this provides us with a check method. The other dial will now give us $SX_2$.

No such check is possible for $SX_1^2$ except on Monroe models equipped with automatic squaring devices.

5.02 Binomial Method

The binomial method takes advantage of the familiar identity

$$(a + b)^2 = a^2 + 2ab + b^2.$$  

It is applicable when the $X$'s are quite small and there are not too many of them. It can be worked on any type of machine, but is handy only on Monroe models equipped with automatic squaring.

In the binomial method we set up two factors in the keyboard at the same time and square. Suppose we have $X_1 = 18$ and $X_2 = 11$; we require $X_1^2$, $X_2^2$ and $X_1X_2$. We set up 18 at the left of the keyboard and 11 at the right; for a ten-bank machine this gives us

18 0 0 0 0 0 0 1 1.

Squaring gives us

3 2 4 0 0 0 0 0 3 9 6 0 0 0 0 0 1 2 1.

At the left we have $324 = 18^2$, at the right $121 = 11^2$. In the middle we have $396 = \frac{1}{2} \times 18 \times 11$. We can thus, by successive squaring, build up $SX_1^2$, $2SX_1X_2$, and $SX_2^2$ in one dial, and $SX_1$ and $SX_2$ in the other. It is of course essential that the numbers be small enough so that the totals do not run together in the dials. Caution: Don't forget to divide the middle number by 2 to get $SX_1X_2$. 


5.03 Punch Card Method

This method is adapted to use with IBM punch card machines. The equipment required is a card punch, a sorter, and a tabulator capable of recording sub-totals ("Major" and "Minor" control). No multiplier is needed; even should a multiplying punch be available, it would not be used for this job.

In order to illustrate the principle involved, let us find the sums of the squares of the integers 1 to 9 inclusive. We arrange them in descending order, and beneath each number write the cumulative sub-total, thus:

<table>
<thead>
<tr>
<th>Numbers</th>
<th>9 8 7 6 5 4 3 2 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sub-totals</td>
<td>9 17 30 35 39 42 44 45 Total 285</td>
</tr>
</tbody>
</table>

Adding together all the sub-totals we get 285, which is equal to 81 + 64 + 49 + 36 + 25 + 16 + 9 + 4 + 1, the sum of the squares of the first nine integers. The reason why this works can be seen easily if we display the sub-totals thus:

| 9 9 9 9 9 9 9 9 9 |
| 9 8 8 8 8 8 8 8 8 |
| 17 7 7 7 7 7 7 7 7 |
| 24 6 6 6 6 6 6 6 6 |
| 30 5 5 5 5 5 5 5 5 |
| 35 4 4 4 4 4 4 4 4 |
| 39 3 3 3 3 3 3 3 3 |
| 42 2 2 2 2 2 2 2 2 |
| 44 1 1 1 1 1 1 1 1 |
| 45 0 0 0 0 0 0 0 0 |

We see that the sum of the sub-totals contains 9 nine times, 8 eight times, and so on.

It is essential that there be as many sub-totals as the largest integer in the series. If any integer is missing, the gap must be filled by a zero — i.e., a blank card. We can find the sum of squares of the first four even numbers thus:

<table>
<thead>
<tr>
<th>Numbers</th>
<th>8 0 6 0 4 0 2 0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sub-totals</td>
<td>8 8 14 14 18 18 20 20 Total 120</td>
</tr>
</tbody>
</table>

Here the missing numbers are represented by zeros. The reason will be clear enough if the sub-totals are analyzed as above.

Total cross-products can be obtained similarly. The multipliers must run from 1 to 9, missing numbers being indicated by zero. The pairs of factors are arranged so that the multipliers run in descending order from 9 to 1. If we want \((3x8) + (2x7) + (8x5) + (4x3) + (6x1)\), we can write

| Multipliers | 8 7 0 5 4 3 0 1 28 |
| Sub-totals   | 8 15 15 20 24 27 27 28 164 |
| Multiplicands| 3 2 0 8 4 0 0 6 23 |
| Sub-totals   | 3 5 5 13 17 17 17 23 100 |

The totals are \(SX_1 = 28, SX_1^2 = 164, SX_2 = 23, SX_1X_2 = 100\). Another run must be made to get \(SX_2^2\).

In practice we begin by punching the data. One card should be used for each set of observations; there will thus be \(n\) cards in all. Suppose now that we want
SX², and that the individual X₂'s run from 1 to 96. We could sort the cards into descending order by X₂, filling in the gaps (if any) with blank cards, then make our run, taking minor sub-totals with each change in the units digit. At the end we should have 96 sub-totals, which when added together would give us SX². In another adding bank we might simultaneously have made totals for X₃, and the sub-totals in that bank would give us SX₂X₃.

It is usually more convenient to sort first from 9 to 0 on the units column of X₂ and make a first run obtaining 10 sub-totals. The last of these is of course SX₂, since it is the total for all the cards; it is not included in summing sub-totals. We may denote the sum of the first nine sub-totals by S₁ — the summation when cards are sorted by the units digit. We now re-sort the cards, this time on the tens digit, and make a second run, obtaining a new set of sub-totals. The last of these will be SX₂ again; the first nine are added to get what we shall call S₂. We now calculate easily

\[ SX² = S₁ + 10S₂. \]

If we have been carrying SX₃ in another bank, we can simultaneously get SX₂X₃ in the same way: the sum of the first nine sub-totals plus ten times the sum of the second nine. If the numbers are not too large, we can run two columns of figures in the same bank. With five adding banks and small numbers it is possible to get SX₁, SX₂, ... SX₁₀, SX₁S₂, ... SX₁X₁₀ all simultaneously, simply by accumulating two columns of figures in each bank.

If X is a three or four figure number, 3 or 4 runs will be required, sorting first on the units, then on the tens, then the hundreds, and so on, using the sub-totals to get respectively S₁, S₂, S₃, ... We shall then have

\[ SX² = S₁ + 10S₂ + 100S₃ + \ldots \]

Not much is usually gained by punching more than 3 figures, and for most purposes 2 should be ample.

The punch card method is useful if there are as many as 100 observations, and is the only practicable method for handling large masses of data. The chief labor item is punching and checking the cards; the sorter and tabulator runs are comparatively minor jobs. If some of the X's are negative, the whole set should be coded to make all measurements positive; the method does not work for negative numbers. If only a few negative values occur, they can be sorted out and dealt with separately, but this expedient is not recommended.

6. Coding

Coding measurements means expressing them in new units, or from a new zero, or both. If our data are in inches and we convert them to feet, we have an example of coding by change of units. If we convert temperature measurements to degrees above or below normal, we are changing the zero — that is, making a translation of the origin. If we convert from Fahrenheit to Centigrade, we change both the unit and the zero point.

The purpose of coding in curve fitting is to give more manageable numbers. While the laws of algebra apply whether numbers are large or small, the arithmetic can frequently be made easier by suitable coding. Suppose for example that we have to calculate a number and its reciprocal. Let the number be 331,758. Its reciprocal is 0.000000301425. If now we adopt new units 100,000 times as big as the old, we get for our two numbers 3.31758 and 0.301425, equivalent to the first two but easier to handle. Again, if we have a set of measurements 11.0065, 11.0101,
14.0017, and 14.0080, we can simply drop the 14's, move the decimal point over, and get 0.65, 1.01, 0.77 and 0.80.

The code most commonly used in statistics is a change of origin such that every measurement in a set is converted to a deviation from the average of the set. Let us adopt the notation:

\[
\begin{align*}
X &= \text{a measurement}, \\
n &= \text{the number of measurements in a set}, \\
\bar{x} &= \text{the mean or average of the } n \text{ measurements}, \\
x &= \text{a coded measurement} = X - \bar{x}.
\end{align*}
\]

It is quite easy to prove that

\[
\begin{align*}
Sx &= S(X - \bar{x}) = 0, \\
Sx^2 &= S(X - \bar{x})^2 = Sx^2 - nx^2.
\end{align*}
\]

The latter formula can take two other forms:

\[
\begin{align*}
Sx^2 &= Sx^2 - \bar{x}Sx \\
Sx^2 &= Sx^2 - \frac{(Sx)^2}{n}.
\end{align*}
\]

All these are obvious if we remember that by definition \(Sx = n \bar{x}\).

If we code all measurements to their means, the \(Sx^2\) of the normal equations go to \(Sx^2\), which on calculating machines is usually easiest computed by (6.03a). The cross products \(SxX_j\) go to \(SxX_j\), and these also can be calculated by formula:

\[
\begin{align*}
SxX_j &= SxX_j - \bar{x}_j(Sx_j) \\
SxX_j &= SxX_j - \frac{(Sx_j)(Sx_j)}{n}
\end{align*}
\]

or any one of several other equivalent forms.

6.1 Reduction to Means by Abbreviated Doolittle Method

All the sums of squares and cross-products of a set can be converted to coded values measured from their means by a simple modification of the Abbreviated Doolittle method.

We begin by arbitrarily defining \(x_1 = 1\) (unity) for all observations. This means that \(Sx_1 = n\) and \(Sx_1x_i = SX_i\). Our normal equations are written in skeleton form, as before, including the check column. We continue with the first section of the forward solution by copying the first normal equation for the row of A's, and divide by \(a_{11}\) to get the row of B's. We next go ahead and obtain \(a_{22}, a_{23}, \ldots\) as usual. Up to this point the work has been exactly as for Table 4.4.03.

The row starting with \(a_{22}\) is, however, carried out to the end, including the check column, and the division of \(a_{23}, \ldots\) by \(a_{22}\) is omitted. Instead, as soon as we have calculated the \(a_{22}\) row we start a new row, obtained in exactly the same way but beginning with \(a_{33}\). The procedure is most clearly shown by example.
Table 6.1.01 Reduction of $a_{ij}$ to Deviations from Mean

\[
\begin{array}{cccccc}
  a_{11} & a_{12} & a_{13} & a_{14} & a_{15} & g_1 & j_1 \\
  a_{22} & a_{23} & a_{24} & a_{25} & g_2 & j_2 \\
  a_{33} & a_{34} & a_{35} & g_3 & j_3 \\
  a_{44} & a_{45} & g_4 & j_4 \\
  a_{55} & g_5 & j_5 \\
\end{array}
\]

\[
\begin{array}{cccccc}
  A_{11} & A_{12} & A_{13} & A_{14} & A_{15} & A_{16} & j_6 \\
  B_{12} & B_{13} & B_{14} & B_{15} & B_{16} & j_7 \\
  S_{22} & S_{23} & S_{24} & S_{25} & g_2 & j_8 \\
  S_{33} & S_{34} & S_{35} & g_3 & j_9 \\
  S_{44} & S_{45} & g_4 & j_{10} \\
  S_{55} & g_5 & j_{11} \\
\end{array}
\]

At this point the Abbreviated Doolittle Solution may be continued in the ordinary way on the S's; the first seven rows are simply ignored. For the computation of the S's we have

\[
S_{22} = a_{22} - A_{12}B_{12} \\
S_{23} = a_{23} - A_{12}B_{13}, \text{ and so on to} \\
S_{33} = a_{23} - A_{13}B_{13} \\
S_{34} = a_{34} - A_{13}B_{14} \\
S_{44} = a_{44} - A_{14}B_{14} \\
\text{and in general} \\
S_{ij} = a_{ij} - A_{1i}B_{1j}.
\]

If we have followed the convention of letting $X_1 = 1$, $A_{11}$ will be equal to $n$, and the B's in the seventh line will be averages. It should be easy to see that the operation leading to the S's is exactly that indicated by (6.03a) and (6.04a).

In order to place before us a numerical example, let us return to the data of Table 4.1.01. There are 10 sets of observations, and the column totals are

\[
352 \quad 43 \quad 74 \quad 3739.90.
\]

We shall proceed to convert all sums of squares and cross products to measurements from the column means, and then solve anew for the b's in terms of these new measurements.
Table 6.1.02  Aldi With Reduction of Sums of Squares, etc.

<table>
<thead>
<tr>
<th></th>
<th>10</th>
<th>352.</th>
<th>43.</th>
<th>74.</th>
<th>3739.9</th>
<th>4218.9</th>
</tr>
</thead>
<tbody>
<tr>
<td>This row has been added</td>
<td>14190.</td>
<td>1626.</td>
<td>2643.</td>
<td>117551.2</td>
<td>166362.2</td>
<td></td>
</tr>
<tr>
<td>Next three lines same as</td>
<td>213.</td>
<td>359.</td>
<td>17174.2</td>
<td>19715.2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Table 4.3.01 (except check column)</td>
<td>652.</td>
<td>28881.2</td>
<td>32609.2</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>Continue as for Aldi for this section</td>
<td>10</td>
<td>352.</td>
<td>43.</td>
<td>74.</td>
<td>3739.9</td>
<td>4218.9</td>
</tr>
<tr>
<td></td>
<td>35.2</td>
<td>4.3</td>
<td>7.4</td>
<td>373.99</td>
<td>421.89</td>
<td></td>
</tr>
<tr>
<td>These rows contain the reduced sums of squares and cross-products</td>
<td>1799.6</td>
<td>112.4</td>
<td>38.2</td>
<td>15906.72</td>
<td>17856.92</td>
<td></td>
</tr>
<tr>
<td></td>
<td>28.1</td>
<td>40.8</td>
<td>104.4</td>
<td>15906.72</td>
<td>17856.92</td>
<td></td>
</tr>
<tr>
<td></td>
<td>10.8</td>
<td>1205.94</td>
<td>1389.34</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Now go ahead with Aldi</td>
<td>1799.6</td>
<td>112.4</td>
<td>38.2</td>
<td>15906.72</td>
<td>17856.92</td>
<td></td>
</tr>
<tr>
<td></td>
<td>.06245832</td>
<td>.02122694</td>
<td>8.83903090</td>
<td>9.92271616</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Solution completed</td>
<td>21.07968</td>
<td>38.41409</td>
<td>1.82233</td>
<td>18.93401</td>
<td>21.75634</td>
<td></td>
</tr>
<tr>
<td></td>
<td>33.58598</td>
<td>4.19688</td>
<td>5.19688</td>
<td>11.28591</td>
<td>12.28591</td>
<td>8.04505</td>
</tr>
</tbody>
</table>

It may cause some surprise that the b's here obtained are not the same as those found previously. The reason for this will become clear as we proceed.

6.2 Coding by Powers of 10

In Table 6.1.02 we note that in order to have five meaningful decimal places in the second section of the forward solution, it is necessary to carry eight in the B row of the first section. For convenience in keeping the computation sheet reasonably neat looking, it is advisable to adopt units such that we do not have very large and very small quantities. There are several methods for doing this, but the simplest is to convert to new units that differ from the old by some factor of 10 or a power of 10.

The thing to remember is that if we divide each \(X_1\) by 10, then \(Sx_1^2\) will be divided by 100. If we also divide each \(X_2\) by 100, then \(Sx_2\) will be divided by 10,000 and \(SX_1X_2\) by 1,000. We can usually decide what power of 10 to use by looking at the diagonal terms, which are all sums of squares. It is convenient to have these diagonal terms somewhere between .1 and 10., and we can always find some even power of 10 to do this. In Table 6.1.02 the first diagonal term in the reduced matrix is 1799.6, and if this is divided by 10,000 we get .17996, a number in the desired range. The second diagonal term is 28.1, which can be divided by 100 to give .281. The same divisor will suffice for the third diagonal term.

We can proceed by first writing down these divisors in a diagonal array so that each corresponds to the term it is to divide. At the same time, we write the square root of each divisor as an index to the corresponding row and column, thus:

\[
\begin{array}{ccc}
100 & 10 & 10 \\
100 & 10000 & \\
10 & 100 & \\
10 & 100 & \\
\end{array}
\]
We next need to decide upon a code for the g's (that is, the $S_{x,y}$). The first of our g's in Table 6.1.02 is 15906.72, and this is the sum of the $x_2y$ cross-products. We have already decided to divide each $x_2$ by 100, and of course $S_{x_2y}$ will be divided by the same quantity, reducing it to 159.0672. Dividing by 100 again will bring the number down in the desired range, and inspection shows that the same factor will serve for the other g's as well. We can now fill out our table.

Table 6.2.01 Factors for Coding

<table>
<thead>
<tr>
<th></th>
<th>100</th>
<th>10</th>
<th>10</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>10,000</td>
<td>1,000</td>
<td>1,000</td>
<td>10,000</td>
</tr>
<tr>
<td>10</td>
<td>100</td>
<td>100</td>
<td>1,000</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>100</td>
<td>1,000</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The entry in each position is the product of the two applicable factors, which appear at the head of each column and at the beginning of each row. There is of course no code for the j column. Applying these coding factors to our problem, we find that in the Abbreviated Doolittle solution the entries are all of approximately the same order of magnitude, and there is no difficulty in carrying seven places of decimals without clumsiness or loss of accuracy.

Table 6.2.02 Doolittle Solution with Coding to Powers of 10

To decode the results -- that is, to convert them into the original units so that the b's will agree with those obtained in Table 6.1.02, we multiply by the y code and divide by the x code. The y code is 100; the x codes are respectively 100, 10 and 10. Performing these multiplications, we get back to the b's of the uncoded solution.

6.3 Coding to Correlation Coefficients

In 6.2 we expressed each measurement in new units which differed from the old by some power of 10. An example would be changing from grams to kilograms, or cents to dollars. Such coding has the advantage that it requires a minimum of computation. Another method of coding that has considerable advantages is to use as the unit of measurement the standard deviation of the observations themselves. This means that most of the observations become numbers between ±2 and ±2 (we assume that the mean is taken as zero). It also has the consequence that all the diagonal entries in our matrix become unity, and all the non-diagonal entries are converted...
into correlation coefficients. The use of this method of coding insures that every entry in the coefficient matrix will be between +1 and -1; ordinarily all the entries will be of the same order of magnitude, and the arithmetic proceeds very smoothly. Moreover, the correlation coefficients are frequently of interest in themselves. An easy adaptation of the Abbreviated Doolittle technique enables us to get the correlation coefficients with little labor.

It is essential to begin with a "reduced" matrix — that is, one in which we have measured all the variables as deviations from the mean. In order to code the $g$ column, we shall require a new number:

\[(6.3.01) \quad S(y - \bar{y})^2 = S_y^2 - \bar{y}S_y\]

(see page 10) \[= 1,547,855.23 - (373.99)(3739.9) = 119,170.029 .\]

The square root of this quantity we shall call $s_5$. We find readily

\[(6.3.02) \quad s_5 = 386.22536 .\]

We are now ready to go ahead with our solution.

<table>
<thead>
<tr>
<th>Table 6.3.03</th>
<th>ADM with Reduction to Correlation Coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reduced sums of squares</td>
<td>1799.6</td>
</tr>
<tr>
<td>and cross-products from Table 6.1.02</td>
<td>28.1</td>
</tr>
<tr>
<td>Square root divisors</td>
<td>42.42169</td>
</tr>
<tr>
<td>Matrix of correlation coefficients</td>
<td>1.</td>
</tr>
<tr>
<td>1.</td>
<td>.75328</td>
</tr>
<tr>
<td>1.</td>
<td>.30559</td>
</tr>
<tr>
<td>Forward solution for ADM begins here.</td>
<td>1.</td>
</tr>
<tr>
<td>1.</td>
<td>.49983</td>
</tr>
<tr>
<td>.75017</td>
<td>.70923</td>
</tr>
<tr>
<td>.94543</td>
<td>.25987</td>
</tr>
<tr>
<td>.32171</td>
<td>***</td>
</tr>
<tr>
<td>1.15491</td>
<td>.80365</td>
</tr>
</tbody>
</table>

For brevity, only five decimals have been carried in the above solution.

There are two new features here. The first is the addition of a row of "Square root divisors". The numbers on this line are the square roots of the diagonal terms of the matrix of reduced sums of squares and cross-products; thus 42.42169 is the square root of 1799.6, and so on. The last entry in the row of square root divisors is $s_5$, calculated in (6.3.02). There is no entry under the check column, hence the asterisks. We shall call the entries in the row of square root divisors $s_2$, $s_3$, $s_4$ and $s_5$.

The numbers in the matrix of correlation coefficients are obtained by dividing each reduced sum of squares or cross-products by two of the s-divisors. Each
diagonal coefficient is thus equal to +1, since it comes from dividing a number twice by its own square root. For each non-diagonal element we have two divisors, the one from the leading column, the other from the column that contains the element; the routine is similar to that for ADI. We have thus

\[(112.4/5.30094)/42.42169 = .49983 ,\]
\[(38.2/10.21763)/42.42169 = .08813 ,\]
\[(40.8/10.21763)/5.30094 = .75328 ,\]
and so on. The double division is easily performed on any of the standard machines.

The second new feature in this solution is the break in the check column. It is not possible to use the same routine for carrying the check column past the line of square root divisors as we have been using, and another device must be used. We begin by dividing 1799.6 by the s-entry beneath it, obtaining of course 42.42169 as the quotient. This is allowed to stand in the machine while we go ahead to divide 112.4 by the s-entry under it, namely 5.30094; we must do this without disturbing the old quotient. On the Friden this is easy, as the new dividend can be inserted by twirling the knobs on the carriage. On the Marchant and Monroe the new dividend has to be added, an operation which of course adds 1 in the quotient dial; this 1 must be taken out by clearing the keyboard and pressing the "minus" key. In either case, we build up the sum of quotients in the machine, obtaining

\[(1799.6/42.42169) + (112.4/5.30094) + (38.2/10.21763)\]
\[+ (1590.6/386.22536) = 108.54919 .\]

This sum must now be divided by the value of s from the leading column; we get

\[108.54919/42.42169 = 2.55881 ,\]

which is the entry for the check column in the first row of the correlation matrix.

For subsequent rows we proceed in the same way, remembering to supply entries omitted because of symmetry. We find

\[(112.4/42.42169) + (28.1/5.30094) + (40.8/10.21763)\]
\[+ (1392.6/386.22536) = 15.54938\]
\[15.54938/5.30094 = 2.93332\]
\[(33.2/42.42169) + (40.8/5.30094) + (104.4/10.21763)\]
\[+ (1205.9/386.22536) = 21.93724\]
\[21.93724/10.21763 = 2.14700 .\]

This kind of check is not quite as good as the type we usually get when we carry along a check column, since it is really no more than a repetition of the arithmetical operations already performed; it is, however, the best check that seems to be available to bridge the gap. Once the new check column totals are obtained, the solution follows the Abbreviated Doolittle routine without change.
7. Constant and Straight Line

The simplest kind of prediction equation (we shall use the term regression equation from now on) arises when we assume that the true value of the quantity being measured is a constant, and that therefore future measurements ought to be the same as present ones, save for random errors. We construct what is called a "mathematical model", thus:

\[ X_i = m + e_i . \]  

Here we regard \( m \) as the true value of the quantity being measured, and \( e_i \) as a chance error that afflicts the \( i \)th measurement. The measurement itself is thus the sum of the two (remember, \( e_i \) may be positive or negative). We shall further assume that the measurements are unbiased -- that is, that each \( e_i \) has the expected value zero. Another assumption we need is that the \( e_i \) are independent (uncorrelated) -- that is, that the error made on (say) the tenth measurement is unaffected by whatever the errors may have been on the preceding nine. Finally, we shall assume that the \( e_i \) have a normal distribution with constant variance; this latter assumption simplifies our work somewhat, though we can use least squares without making it.

The least squares principle now requires that the quantity

\[ S(X_i - m)^2 \]

be as small as possible. Differentiating with respect to \( m \), we obtain readily

\[ m = \frac{\sum X_i}{n} , \]

the equation of the arithmetic mean \( \bar{x} \). We see now that the arithmetic mean is a special case of a least squares solution.

One more point. Equation (7.03) can be written

\[ X_1 + X_2 + X_3 + \ldots + X_n = nm , \]

whence \( nm = Z_1 \) as defined in (3.06) and elsewhere. We have thus \((n - 1)\) degrees of freedom to use for the computation of other statistics. We say that the data are subject to a single linear restriction (that imposed by (7.03)).

Instead of assuming that the quantity being measured is constant, we may assume that it varies in some regular way. The simplest such assumption is that we have a straight line relationship. If moreover we are sure that the straight line must pass through the origin, our mathematical model becomes

\[ y_i = b X_i + e_i , \]

where, as before, the \( e_i \) are assumed to be random errors, normally distributed with constant variance and expectation zero. Our task is to estimate \( b \), and the least squares criterion requires that

\[ S(bX_i - y_i)^2 \]

be a minimum. Differentiating with respect to \( b \) and proceeding as usual we get

\[ b = \frac{(\sum X_i y_i)}{(\sum X_i^2)} . \]

We have a change of notation here, the predicted quantity being denoted by \( y \) (in
(7.01) it was denoted by $X$) and the estimated quantity being now the regression coefficient $b$ instead of the mean value $m$.

Note: Better usage would be to let the Greek letter beta stand for the true (unknown) value of the coefficient and $b$ for the estimate. This is difficult in mimeographed copy when the typewriter has no Greek letter symbols, and we shall accordingly use $b$ for both, unless some ambiguity arises that is not resolved by the context.

In (7.05) we assume that the line of regression passes through the origin. If we remove this restriction, the equation of our straight line will contain a constant term; that is, it will take the form

$$Y = b_1 + b_2 X.$$  

(7.08)

There is some gain in simplicity of notation if we introduce a dummy variable $X_1$ always and identically equal to unity. Equation (7.08) can then be written

$$Y = b_1 X_1 + b_2 X_2.$$  

(7.09)

where $X_2$ is the $X$ of (7.08). Clearly, if $X_1$ is always equal to 1, then $b_1 X_1$ will be the same as $b_1$. We note also that $X_1$ is always 1, $X_1 X_2$ is the same as $X_2$, and that therefore $S X_1 = n$, the number of observations, and $S X_1 X_2 = S X_2$, $S X_1 Y = S y$.

To satisfy the least squares condition, following (4.05), we must find $b_1$ and $b_2$ such that

$$S(Y - y)^2 = S(1_1 X_1 + b_2 X_2 - y)^2.$$  

(7.10)

is a minimum. As usual, we find the partial derivatives with respect to $b_1$ and $b_2$ and set them equal to zero. (Remember that the $X$'s are not variables here; they are the observed data.) We obtain for the normal equations

$$2 S X_1 (b_1 X_1 + b_2 X_2 - y) = 0,$$

$$2 S X_2 (b_1 X_1 + b_2 X_2 - y) = 0,$$

which after obvious rearrangement become

$$b_1 S X_1^2 + b_2 S X_1 X_2 = S X_1 Y,$$

$$b_1 S X_1 X_2 + b_2 S X_2^2 = S X_2 Y.$$  

(7.11)

This solution is valid for any $X_1$ and $X_2$; but if we have adopted the convention that $X_1$ is identically unity, we may write

$$n b_1 + b_2 S X_2 = S y,$$

$$b_1 S X_2 + b_2 S X_2^2 = S X_2 Y,$$

(7.12)

from which by elementary methods

$$b_1 = \frac{S y S X_2 - S X_2 S X_2 Y}{n S X_2^2 - (S X_2)^2}, \quad b_2 = \frac{n S X_2 Y - S X_2 S y}{n S X_2^2 - (S X_2)^2}.$$  

(7.13)
7.1 Examples of Straight Regression Line

Ex. 1 A bottle filling machine is supposed to put one pint of liquid into each bottle. In order to check the performance of the machine over a period of time we take specimen bottles at half-hour intervals and record "over" or "short" in any suitable units. Over a three-hour period we obtain the following data.

<table>
<thead>
<tr>
<th>Time</th>
<th>Amount Over or Short</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:30</td>
<td>+ 21</td>
</tr>
<tr>
<td>9:00</td>
<td>+ 5</td>
</tr>
<tr>
<td>9:30</td>
<td>- 2</td>
</tr>
<tr>
<td>10:00</td>
<td>- 11</td>
</tr>
<tr>
<td>10:30</td>
<td>- 30</td>
</tr>
<tr>
<td>11:00</td>
<td>- 15</td>
</tr>
<tr>
<td>11:30</td>
<td>- 31</td>
</tr>
</tbody>
</table>

What method of analysis shall we apply?

We can of course calculate the average of our seven measurements, obtaining \( y = -9 \). But does this average by itself have any meaning? Referring to the first paragraph of (7) we recall that the calculation of such an average involves assuming that we expect future measurements to be the same save for chance errors. But a glance at the data shows at once that the mean fill is changing with time, and we should clearly not expect future measurements to be the same as these. The mere computation of an average is thus no more than a meaningless exercise in arithmetic.

One might be tempted to say "At any rate, the average does summarize the data at hand." This too is a fallacy. Suppose our observations had occurred in the order

\[ + 5 - 30 - 2 - 31 + 21 - 11 - 15. \]

Since nothing has been changed but the order, our mean value will be the same as before. But since there is now no evidence of a linear trend, we may feel fairly confident that future observations will be somewhere near the observed mean. This illustration shows that the information contained in the data depends not merely upon their numerical values, but also on the order in which they occur. Since the mean depends only upon the numbers, it cannot be said truly to summarize the data.

We agree, then, that computing the mean is not a good way to analyse these data. Shall we fit a straight line that passes through the origin? This would imply that our process had been so adjusted that at zero time, the deviation from standard is zero. This is obviously not the case. If a straight line can represent the data at all, there must be a constant term. We accordingly apply the methods appropriate to (7.08).

It is convenient to rewrite the data in tabular form showing \( X_1 \) and the various squares and cross-products which enter into the normal equations. At the same time we may code the time data to half-hour units, taking 8:30 (the starting point) as zero. This leads to the arrangement of (7.1.02).

Note: In practice these squares and cross-products would be accumulated in a machine following (5.01) or (5.02); the individual listing here is for teaching purposes only, to clarify the procedure by showing each step.
(7.1.02) \[
\begin{array}{cccccc}
X_1 & X_2 & X_2^2 & y & X_2y & y^2 \\
1 & 0 & 0 & +21 & 0 & 1 \\
1 & 1 & 1 & +5 & +5 & 25 \\
1 & 2 & 4 & -2 & -4 & 4 \\
1 & 3 & 9 & -11 & -33 & 121 \\
1 & 4 & 16 & -30 & -120 & 900 \\
1 & 5 & 25 & -45 & -225 & 225 \\
1 & 6 & 36 & -31 & -186 & 961 \\
7 & 21 & 91 & -63 & -413 & 2677 \\
\end{array}
\]

Referring back to (7.11) and (7.12) we see that our normal equations are

\[
\begin{align*}
7b_1 + 21b_2 &= -63 \\
21b_1 + 91b_2 &= -413
\end{align*}
\]

whence by elementary methods

\[
\begin{align*}
b_1 &= +15 \\
b_2 &= -8
\end{align*}
\]

Our regression equation is thus

\[
Y = 15 - 8X.
\]

* * *

Ex. 2 The amount of liquid that flows through an orifice under constant pressure is a linear function of the time. If we are filling bottles, the longer the time allowed, the more liquid will flow. We may try to estimate the rate of flow by measuring the amount at different times, obtaining data something like these:

(7.1.06) \[
\begin{array}{cccc}
\text{Time (seconds)} & \text{Volume (cc)} \\
1 & 117.0 \\
2 & 236.5 \\
3 & 354.3 \\
4 & 471.3 \\
5 & 590.5 \\
6 & 708.4
\end{array}
\]

\[n = 6 \quad S\!X = 21 \quad S\!X^2 = 91 \quad S\!Xy = 10741. \quad S\!y = 2478
\]

In actually carrying out this experiment we should need to avoid some obvious pitfalls. Thus, our six volumes would need to be determined by six independent experiments; we could not, for example, read volumes during a single run at six consecutive one-second intervals. (Such data would not be independent, since each measurement would be subject, not only to its own errors, but also to errors made for preceding measurements.)

* * *

Again, some knowledge of the chief sources of error would be highly desirable, since simple least squares methods presuppose uniform variance for all measurements. If our chief errors are those introduced at the moments of starting and stopping, we may have approximately uniform variance, since each measurement involves one start and one stop. But if errors tend to build up more or less continuously during the run, it may be more realistic to assume that the variance is proportional
to the value of $y$ -- that is, that errors tend to be a fixed percentage rather than a fixed amount. If this is the case, we can still solve the problem by using suitable weights; we shall look at the subject later. For the present we shall assume uniform variance, applying the method appropriate to (7.05), since obviously the line passes through the origin. Formula (7.07) gives at once

$$(7.1.07) \quad b = \frac{SXY}{SX^2} = \frac{10741}{91} = 118.03 \text{ (to six decimals, 118.032967).}$$

The reason for including a value of $b$ to so many decimals will appear shortly.

8. Estimation of Errors

For the case of (7.01), in which we assume that the quantity being measured is constant save for chance errors, we are accustomed to using $S(X - \bar{X})^2$ to estimate the amplitude of the errors. In the same way we use

$$SV^2 = S(Y - y)^2$$

to estimate the errors in least squares. In (7.01), (7.05), and more generally in (4.02), we assume that each $y_i$ is afflicted with a chance error $e_i$. The variance of these errors is of course a measure of the precision with which the $y_i$'s are ascertained; see the discussion of errors of ascertainment in Section 2. For each $y_i$ we can calculate a $\hat{y}_i$ by least squares; this calculated $\hat{y}$ bears the same logical relationship to the corresponding $y$ as does the mean $\bar{x}$ to the individual measurements. We define

$$(8.01) \quad v_i = y_i - \hat{y}_i ;$$

$v_i$ is called a residual. It is of course not the same as the error $e_i$, but under our assumptions it is an unbiased estimate of $e_i$, and we can estimate the variance of the $e_i$'s from $SV^2$. The appropriate formula is

$$(8.02) \quad s^2 = \frac{SV^2}{D.F.},$$

where D.F. indicates the degrees of freedom available for the estimate. In (7.03) and (7.07) we have calculated single statistics ($\bar{x}$ in the first, $b$ in the second) and our D.F. $= n-1$. In (7.13) we calculated two statistics, $b_1$ and $b_2$, leaving n-2 D.F. In general, in any least squares problem in which we calculate $p$ regression coefficients $b_1, b_2, \ldots b_p$, we shall have $n-p$ D.F.

Let us look at the problem of (7.1.02) and compare the observed values of $y$ with those calculated from (7.1.05).

$$(8.03) \quad \begin{array}{cccc}
X_2 & y (obs) & Y (calc) & v^2 \\
--- & --- & --- & --- \\
0 & +21 & +15 & 36 \\
1 & +5 & +7 & 4 \\
2 & -2 & -1 & 1 \\
3 & -11 & -9 & 4 \\
4 & -30 & -17 & 169 \\
5 & -15 & -25 & 100 \\
6 & -31 & -33 & 4 \\
& -63 & -63 & 318 \\
\end{array}$$

Here $SV^2 = 318$. We had 7 observations and fitted two constants, which leaves
us \(7 - 2 = 5\) D.F. Our estimate of the variance is

\[
(8.01) \quad s^2 = \frac{318}{5} = 63.6 ,
\]

which gives an estimated standard error \(s = 8\) minus. This standard error applies to the observed value of \(y\); it is a measure of the error of ascertainment.

We recall that in calculating \(S(X - \bar{X})^2\) it was not necessary to obtain the individual differences. Instead, we used the formula

\[
S(X - \bar{X})^2 = SX^2 - \bar{X}^2SX .
\]

Analogous formulas are available for least squares problems. The general formula is

\[
(8.05) \quad S(Y - y)^2 = Sy^2 - b_1SX_1y - b_2SX_2y - \ldots - b_pSX_py.
\]

For the present problem, we have

\[
(8.06) \quad S(Y - y)^2 = Sy^2 - b_1SX_1y - b_2SX_2y \\
= 2677 - (15)(-63) - (-8)(-413) \\
= 2677 + 945 - 3304 \\
= 318 , \text{ as before.}
\]

We note incidentally from (8.03) that \(Sy = SY\). It is sometimes said that this always happens, but the statement is not true. The true statement is that we have always

\[
(8.07) \quad SX_1y = SX_1Y
\]

and since \(Y = y + v\) it follows readily that

\[
(8.08) \quad SX_1v = 0 .
\]

In (8.03) \(X_1 = 1\), and by (8.07)

\[
SX_1y = SX_1Y ,
\]

that is,

\[
SY = SY .
\]

This equation will hold whenever our regression equation contains a constant term. It is easy to verify in (8.03) that \(SX_2y = SX_2Y\).

In the example of (7.1.06) let us take \(b = 118.03\) (rounding to two decimals).

\[
(8.09) \quad \begin{array}{cccc}
X & y (obs) & y (calc) & v \quad v^2 \\
1 & 117.0 & 118.03 & +1.03 & 1.0609 \\
2 & 236.5 & 236.06 & -.54 & .2916 \\
3 & 354.3 & 354.09 & -.21 & .0441 \\
4 & 471.3 & 472.12 & +.82 & .6724 \\
5 & 590.5 & 590.15 & -.35 & .1225 \\
6 & 708.4 & 708.18 & -.22 & .0484 \\
\hline & 2478.0 & 2478.63 & & 2.1419 = Sv^2 .
\end{array}
\]
Since we have fitted only one constant, we have five D.F., and readily compute
$s^2 = .128$, $s = .66$ about. We note that $S_y$ is not equal to $S_Y$; but it is easy
to verify that, save for rounding errors, $S_Xy = S_XY$ and $S_Xv = 0$.

The effects of rounding errors in least squares work is sometimes startling.
Suppose we use our value $b = 118.03$ to calculate $S_v^2$ by formula:

$$S_v^2 = S_y^2 - bS_Xy$$

$$= 1,267,794.24 - (118.03)(10711)$$

$$= 34.01$$

which does not agree very well with the 2.11 obtained by direct computation. But
if we write

$$S_v^2 = 1,267,794.24 - (118.032967)(10711)$$

$$= 2.11153$$

we come a bit closer. The point is important enough to warrant a little elaboration.
Let us indicate our subtraction thus:

$$S_y^2 = \begin{array}{c}
1,267,794.24 \\
(118.032967)(10711) = 1,267,792.09857 \\
S_v^2 = 2.11153
\end{array}$$

We have used 9 significant figures in our value of $b$ (really 10, as the next figure
is zero) and accordingly have the same number of significant figures in the subtrahend.
The result is that our difference is accurate to the third decimal, which
 corresponds to the 10th significant figure of the subtrahend. If we use only two
decimals for $b$, we get

$$S_y^2 = \begin{array}{c}
1,267,794.24 \\
(118.03)(10711) = 1,267,760.23 \\
S_v^2 = 34.01
\end{array}$$

the subtrahend being accurate to five figures only, and the difference to none at
all. It is of some interest to show how the calculation of $S_v^2$ from the formula
is affected by the number of decimals carried in $b$.

<table>
<thead>
<tr>
<th>No. of Decimals</th>
<th>Value of $b$</th>
<th>Formula Value for $S_v^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>118.0</td>
<td>356.24</td>
</tr>
<tr>
<td>2</td>
<td>118.03</td>
<td>34.01</td>
</tr>
<tr>
<td>3 or 4</td>
<td>118.0330</td>
<td>1.787</td>
</tr>
<tr>
<td>5</td>
<td>118.03297</td>
<td>2.10923</td>
</tr>
<tr>
<td>6 or 7</td>
<td>118.0329670</td>
<td>2.11153</td>
</tr>
<tr>
<td>8</td>
<td>118.03296703</td>
<td>2.1113077</td>
</tr>
</tbody>
</table>

Exact value of $S_v^2$ to 8 places $2.11109890$

In the last complete paragraph on page 11 we have already mentioned the advisability
in least squares computations of carrying as many decimals as our machine will take.
We shall meet with other examples as we proceed, but the present one should suffice
to admonish whosoever would be admonished.
9. Use of Inverse Matrix in Least Squares

Before we go further in our study of least squares, we must examine an approach and a notation which offer considerable advantages in simplifying the mathematical work. We have already, in (9.06), introduced the normal equations,

\[ b_1 S_{X_1}^2 + b_2 S_{X_1 X_2} + \ldots + b_p S_{X_1 X_p} = S_{X_1 y}, \]
\[ b_1 S_{X_1 X_2} + b_2 S_{X_2} + \ldots + b_p S_{X_2 X_p} = S_{X_2 y}, \]
\[ \ldots \ldots \]
\[ b_1 S_{X_1 X_p} + b_2 S_{X_2 X_p} + \ldots + b_p S_{X_p}^2 = S_{X_p y}. \]

Using a more compact notation as suggested in (4.4.01) and (4.4.02) we may write

\[ (9.01) \quad b_1 a_{11} + b_2 a_{12} + \ldots + b_p a_{1p} = g_1, \]
\[ b_1 a_{21} + b_2 a_{22} + \ldots + b_p a_{2p} = g_2, \]
\[ \ldots \ldots \]
\[ b_1 a_{p1} + b_2 a_{p2} + \ldots + b_p a_{pp} = g_p, \]

where \( S_{X_i X_j} = a_{ij}, \) \( S_{X_i y} = g_i. \)

The array

\[ (9.02) \quad a_{11} \quad a_{12} \quad \ldots \quad a_{1p} \]
\[ a_{21} \quad a_{22} \quad \ldots \quad a_{2p} \]
\[ \ldots \ldots \]
\[ a_{p1} \quad a_{p2} \quad \ldots \quad a_{pp} \]

is called the a-matrix (sometimes the information matrix, though strictly speaking the information matrix would include the column of g's also). We note that the a-matrix is symmetrical; that is, \( a_{ij} = a_{ji}, \) since both are equal to \( S_{X_i X_j}. \) We may if we like regard the a's as elements of a determinant, and the value of this determinant we shall designate by \( D. \)

The solutions of the equations of (9.01) can be readily indicated in determinant form; for example, we have

\[ (9.03) \quad b_1 = \frac{g_1}{D} \begin{vmatrix} a_{11} & a_{12} & \cdots & a_{1p} \\ g_2 & a_{22} & \cdots & a_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ g_p & a_{p2} & \cdots & a_{pp} \end{vmatrix}. \]

The numerator of (9.03) is a determinant, and we can if we like expand it by the elements of its first column -- that is, the g's -- obtaining
where by $A_{ij}$ we mean the cofactor of the element $a_{ij}$ in $D$. (The cofactor is the same as the minor, save that it includes the appropriate sign: $+ \text{ if } i+j \text{ is even},$ $- \text{ if } i+j \text{ is odd}.$) We may now write (9.03) thus:

$$(9.05) \quad b_1 = \frac{a_{11}}{D} + \frac{a_{21}}{D} + \ldots + \frac{a_{p1}}{D}.$$  

If for the fraction $\frac{A_{ij}}{D}$ we substitute the symbol $c_{ij}$, we have

$$(9.06) \quad b_1 = c_{11}e_1 + c_{21}e_2 + \ldots + c_{p1}e_p,$$

or more compactly and generally,

$$(9.07) \quad b_j = \sum c_{ij}e_i.$$

It is apparent that for every $a_{ij}$ there is a corresponding $c_{ij}$, and the complete array, written

$$(9.08) \quad c_{11} \quad c_{12} \ldots \quad c_{1p}$$
$$c_{21} \quad c_{22} \ldots \quad c_{2p}$$
$$\ldots$$
$$c_{p1} \quad c_{p2} \ldots \quad c_{pp}$$

is called the inverse of the matrix of the $a_{ij}$; more briefly, the inverse matrix or the $c$-matrix.

As we shall see, the Abbreviated Doolittle Method is readily adapted to the computation of the inverse matrix, from which, if we so desire, we can obtain the $b$'s with little trouble by using the equations (9.07). The chief importance of the $c$-matrix is not, however, that it leads to simpler computation of the $b$'s; in fact, it hardly does. In the next section we shall discover some better uses for the inverse matrix.

10. Reliability of Least Squares Estimates

In least squares we assume that every $y_i$ is afflicted with an error $e_i$, and that the residual $(y_i - \hat{y}_i) = v_i$ is an unbiased estimate of $e_i$. We have already learned to estimate the variance of the errors $e_i$ from the formula

$$(10.01) \quad s^2 = \frac{\sum v^2}{n-p}.$$  

We now turn to an examination of the $b$'s. Since the $b$'s are calculated from the $y$'s, they too will be subject to chance errors and will have a variance. It can be shown that the variance of a regression coefficient $b_i$ is given by the formula

$$(10.02) \quad V(b_i) = c_{ii}s^2,$$

where $s^2$ is found from (10.01) and $c_{ii}$ is a diagonal element of the $c$ matrix.
The proof that (10.02) gives the variance of $b_i$ will be found in the mathematical appendix; the student who prefers to take it as proved may do so. But in order to use the fact we require some method for obtaining the $c$-matrix. As has been intimated, the Abbreviated Doolittle Method can be made to serve.

10.1 Computation of the Inverse Matrix by the Abbreviated Doolittle Method

We follow the pattern and notation of (10.0.03), but omit the column of $g$'s. In actual least squares work it will usually be well to carry the $g$'s along, but to do so here would clutter up the problem.

Table 10.1.01 The Abbreviated Doolittle Method for Inverse Matrix

The first $n$ rows contain the statement of the problem, i.e., the coefficients of the normal equations.

\[
\begin{array}{cccccc}
  a_{11} & a_{12} & a_{13} & a_{14} & a_{15} & j_1 \\
  a_{22} & a_{23} & a_{24} & a_{25} & a_{26} & j_2 \\
  a_{33} & a_{34} & a_{35} & a_{36} & a_{37} & j_3 \\
  a_{44} & a_{45} & a_{46} & a_{47} & a_{48} & j_4 \\
  a_{55} & a_{56} & a_{57} & a_{58} & a_{59} & j_5 \\
\end{array}
\]

Forward Solution begins here

\[
\begin{array}{cccccc}
  A_{11} & A_{12} & A_{13} & A_{14} & A_{15} & j_1 \\
  B_{12} & B_{13} & B_{14} & B_{15} & j_2 \\
  A_{22} & A_{23} & A_{24} & A_{25} & j_3 \\
  B_{23} & B_{24} & B_{25} & j_4 \\
  A_{33} & A_{34} & A_{35} & j_5 \\
  B_{34} & B_{35} & j_6 \\
  A_{44} & A_{45} & j_7 \\
  B_{45} & j_8 \\
  A_{55} & j_9 \\
\end{array}
\]

Forward solution ends here

The inverse matrix

\[
\begin{array}{cccccc}
  c_{11} & c_{12} & c_{13} & c_{14} & c_{15} \\
  c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\
  c_{33} & c_{34} & c_{35} & c_{36} & c_{37} \\
  c_{44} & c_{45} & c_{46} & c_{47} & c_{48} \\
  c_{55} & c_{56} & c_{57} & c_{58} & c_{59} \\
\end{array}
\]

The forward solution is exactly as before, save that we now write down $j_{1l}$, which was omitted in (10.0.03). This done, we turn at once to the computation of the $c$'s, beginning at the lower right hand corner, in this case with $c_{55}$. We next get $c_{45}$, then $c_{35}$, and so on up the last column until it is complete; then we compute the next lower diagonal entry, in this case $c_{4l}$, and proceed up the fourth column. The last entry calculated is $c_{1l}$.
Equations for computing the c's follow. Note that each diagonal c starts with the reciprocal of the corresponding A; in fact, \( c_{55} \) is simply the reciprocal of \( A_{55} \). Non-diagonal c's are obtained by multiplying the c's already obtained in the same column by the appropriate string of B's.

\[
(10.1.02) \quad c_{55} = \frac{1}{A_{55}} .
\]

\[
c_{15} = -B_{45} c_{55} \quad \text{(note introduction of minus sign here)} .
\]

\[
c_{35} = -B_{34} c_{45} - B_{35} c_{55}
\]

\[
c_{25} = -B_{23} c_{35} - B_{24} c_{45} - B_{25} c_{55}
\]

\[
c_{15} = -B_{12} c_{25} - B_{13} c_{35} - B_{14} c_{45} - B_{15} c_{55} .
\]

This completes the column. For a partial check, we can calculate

\[
a_{15} c_{15} + a_{25} c_{25} + a_{35} c_{35} + a_{45} c_{45} + a_{55} c_{55} = 1,
\]

or so it should. This check is better than nothing, but is not fool proof.

\[
c_{14} = \frac{1}{A_{14}} - B_{14} c_{45} 
\]

\[
c_{34} = -B_{34} c_{45} - B_{35} c_{55}
\]

\[
c_{24} = -B_{23} c_{34} - B_{24} c_{45} - B_{25} c_{55}
\]

\[
c_{14} = -B_{12} c_{24} - B_{13} c_{34} - B_{14} c_{45} - B_{15} c_{55}
\]

completing the fourth column. (We regard \( c_{15} \) as belonging to this column, though we do not copy it; the c matrix, like the a matrix, is symmetrical.) We may calculate for a check

\[
a_{14} c_{14} + a_{24} c_{24} + a_{34} c_{34} + a_{44} c_{44} + a_{54} c_{54} = 1, \text{ or nearly.}
\]

The remaining equations are given without further comment.

\[
c_{33} = \frac{1}{A_{33}} - B_{34} c_{43} - B_{35} c_{53}
\]

\[
c_{23} = -B_{23} c_{33} - B_{24} c_{43} - B_{25} c_{53}
\]

\[
c_{13} = -B_{12} c_{23} - B_{13} c_{33} - B_{14} c_{43} - B_{15} c_{53}
\]

\[
a_{13} c_{13} + a_{23} c_{23} + a_{33} c_{33} + a_{43} c_{43} + a_{53} c_{53} = 1, \text{ or nearly.}
\]

\[
c_{22} = \frac{1}{A_{22}} - B_{23} c_{32} - B_{24} c_{42} - B_{25} c_{52}
\]

\[
c_{12} = -B_{12} c_{22} - B_{13} c_{32} - B_{14} c_{42} - B_{15} c_{52}
\]

\[
a_{12} c_{12} + a_{22} c_{22} + a_{23} c_{32} + a_{24} c_{42} + a_{25} c_{52} = 1, \text{ or nearly.}
\]

\[
c_{11} = \frac{1}{A_{11}} - B_{12} c_{21} - B_{13} c_{31} - B_{14} c_{41} - B_{15} c_{51}
\]

\[
a_{11} c_{11} + a_{12} c_{12} + a_{13} c_{13} + a_{14} c_{14} + a_{15} c_{15} = 1, \text{ or nearly.}
\]

\[
a_{15} c_{11} + a_{25} c_{12} + a_{35} c_{13} + a_{45} c_{14} + a_{55} c_{15} = 0, \text{ or nearly.}
\]

All sums of products similar to the last should be zero.
10.2 Numerical Example of Abbreviated Doolittle Solution for Inverse Matrix

We use the problem of (6.2.02), omitting the column of g's.

\[
\begin{bmatrix}
0.17796 & 0.1124 & 0.0382 & 0.33056 \\
0.281 & 0.108 & 0.8014 & 1.044 \\
1.044 & 1.1902 & & \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
0.17796 & 0.1124 & 0.0382 \\
0.1124 & 0.281 & 0.6215332 \\
0.0382 & 0.2122694 & 1.3368526 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
0.17796 & 0.1124 & 0.0382 \\
0.1124 & 0.281 & 0.6215332 \\
0.0382 & 0.2122694 & 1.3368526 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
2.107968 & 0.3311409 & 1.8223280 \\
1.8223280 & 2.8223203 & & \\
0.3311409 & 1.8223280 & 2.8223203 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
9.9600709 & -7.9868959 & 2.7568761 \\
-7.9868959 & 14.6315768 & -5.4251146 \\
2.7568761 & -5.4251146 & 2.9774258 \\
\end{bmatrix}
\]

The c matrix

\[
\begin{bmatrix}
.0332(2.7568761) + (.08)(-5.4251146) + (1.044)(2.9774258) = .9999999 \\
(.1124)(-7.9868959) + (.281)(14.6315768) + (.0382)(-5.4251146) = 1.0000007 \\
(.17796)(-9.9600709) + (.1124)(-7.9868959) + (.0382)(2.7568761) = .9999999 \\
(.0382)(-9.9600709) + (.1124)(-7.9868959) + (1.044)(2.7568761) = .0000002 \\
\end{bmatrix}
\]

The last four equations provide a partial check. In this example it is not difficult to evaluate the determinant of the a's, as well as all the minors, and thus get values of the c's directly. If we do this we obtain for the c-matrix

\[
\begin{bmatrix}
9.9600696 & -7.9868926 & 2.7568761 \\
-7.9868926 & 14.6315768 & -5.4251146 \\
2.7568761 & -5.4251146 & 2.9774258 \\
\end{bmatrix}
\]

from which we see that the results obtained by the preceding method are in no case quite accurate to the sixth decimal, while the error in \( c_{22} \) would be enough to alter the rounded value to five decimals.

We may if we wish calculate the b's using (9.07); the g's are from (6.2.02)

\[
b_1 = (9.9600709)(1.590672) + (-7.9868959)(1.39263) + (2.7568761)(1.20594) = 8.0450428 \\
b_2 = (-7.9868959)(1.590672) + (14.6315768)(1.39263) + (-5.4251146)(1.20594) = 1.1285959 \\
b_3 = (2.7568761)(1.590672) + (-5.4251146)(1.39263) + (2.9774258)(1.20594) = 1.1285967
\]

We note that the inverse matrix method has given slightly less accurate results, and
11. Straight Line with Orthogonal Coefficients

In fitting the straight line of (7.08) we took the measurements on \( X \) as they came -- that is, without coding. There is a considerable advantage in transforming these \( X \)'s to deviations from their own mean. Our line of regression will then be

\[
Y = b_1 + b_2(X - \bar{x}).
\]

If we write the small letter \( x \) to represent \((X - \bar{x})\) -- that is, the deviation of a particular measurement from the mean of the set -- (11.01) becomes

\[
Y = b_1 - b_2x.
\]

This notation, using \( x \) to represent \((X - \bar{x})\), is convenient and will be adopted in this monograph. The capital \( X \) will then always stand for original measurements, or measurements referred to an arbitrary origin. We note that the sum of the \( x \)'s is always zero, for

\[
Sx_i = S(X_i - \bar{x})
\]

\[
= X_1 - \bar{x} + X_2 - \bar{x} + \ldots + X_n - \bar{x}
\]

\[
= X_1 + X_2 + \ldots + X_n - n\bar{x} = 0.
\]

We recall also the equivalence

\[
Sx^2 = S(X - \bar{x})^2 = Sx^2 - \bar{x}(Sx).
\]

Using \( x \) instead of \( X \), we find our normal equations much simplified:

\[
b_1 = \frac{Sy}{Sx^2} = \frac{Sxy}{Sx^2},
\]

whence

\[
b_1 = \frac{Sy}{n} = \bar{y}
\]

\[
b_2 = \frac{Sxy}{Sx^2}.
\]

The important point here is that \( b_1 \) and \( b_2 \) are defined by two separate equations, not by a pair of simultaneous equations in two unknowns. Thus, \( b_1 \) and \( b_2 \) are connected only through the right-hand terms of (11.05), viz., \( Sy \) and \( Sxy \). If \( Sy \) and \( Sxy \) are independent, it follows that \( b_1 \) and \( b_2 \) must be so also. But it is easy to see that \( Sy \) and \( Sxy \) are orthogonal. Let us write

\[
Z_1 = Sy = y_1 + y_2 + \ldots + y_n
\]

\[
Z_2 = Sxy = x_1y_1 + x_2y_2 + \ldots + x_ny_n.
\]

The sum of products of corresponding coefficients is \( Sx = 0 \); the \( Z \)'s are therefore orthogonal, and will be independent if the \( y \)'s are (which is assumed).

It is worth noticing that if we use \( X \) instead of \( x \), this property is lost. Starting with (11.01) we get

\[
Y = b_1 + b_2(X - \bar{x})
\]

\[
= (b_1 - b_2\bar{x}) + b_2X.
\]

The constant term now contains both \( b_1 \) and \( b_2 \), and is independent of \( b_2 \) only when \( \bar{x} = 0 \).
The a-matrix from (11.05) is

\[
\begin{pmatrix}
 n & 0 \\
 0 & Sx^2 \\
\end{pmatrix}
\]

and its inverse can be written down at sight; it is

\[
\begin{pmatrix}
 1/n & 0 \\
 0 & 1/Sx^2 \\
\end{pmatrix}
\]

We may use (10.02) to find the error of the b's:

\[
\begin{align*}
 V(b_1) &= c_{11}s^2 = s^2/n \\
 V(b_2) &= c_{22}s^2 = s^2/Sx^2 \\
 V(Y_1 + Y_2) &= V(Y_1) + V(Y_2) \quad \text{if } Y_1 \text{ and } Y_2 \text{ are independent;} \\
 V(kY) &= k^2V(y) \quad \text{where } k \text{ is any constant.}
\end{align*}
\]

Since \( b_1 \) and \( b_2 \) are independent, we can estimate the variance of our calculated values \( Y \):

\[
V(Y_0) = V(b_1 + b_2x_0)
\]

\[
= V(b_1) + x_0^2V(b_2)
\]

\[
= \frac{s^2(Sx^2 + nx_0^2)}{nSx^2}
\]

If \( x_0 = \bar{x} \), this gives us back the variance of the mean. We notice that \( V(Y) \) is a minimum for this case, and that any predicted \( Y \) will become less and less precise as the corresponding value of \( x \) is farther from the mean.

12. Errors in Straight Line Regression: Recapitulation

The subject of variance of least squares linear estimates is important enough to justify us in pausing here to take stock. In the first place, we distinguish at least three kinds of error.

Our least squares solution is based on a set of measurements on the dependent variable \( y \), which is subject to an error \( e \). This is an error of ascertainment. It arises because our methods of measuring \( y \) are subject to error, and because \( y \) itself may be imperfectly defined in our problem. The error of \( y \) is measured by \( V(y) \), and our estimate of it is

\[
V(y) = s^2 = Sv^2/(n - 2) .
\]

The validity of this estimate rests upon the basic assumptions, which are

12.02 a. The errors of \( y \) are all mutually independent;
   b. The variance of the errors is the same for all \( y \)'s;
   c. \( X \) is known substantially without error, and
   d. The true line of regression is really straight.
How often are these assumptions satisfied? Probably not often more than to a moderate degree of approximation. As we have seen, exactness is an illusion, and the final judgment of any method must be on results. Certainly the method of least squares has been widely applied, presumably with enough success to justify its continuance.

If (a) does not hold, we can sometimes reduce the correlation between errors by good design. If (b) is false, we can sometimes use weighting techniques, or some kind of transformation of the y's. If (c) is false, our line of regression will still be valid, but of course our estimate of the error of y will be inflated due to the error in X. Finally, if (d) is false our remedy is to seek the true regression line and use it. This may be difficult or impossible, and one of the most obscure problems in statistics is in fact that of testing the appropriateness of our mathematical models.

The errors of $b_1$ and $b_2$ are errors of estimation, as is the error of $s^2$. In the orthogonal case $b_1 = \bar{y}$, an estimate of the unknown true mean of the y's. The slope of the line is $b_2$, an estimate of the rate of change in y relative to X. The estimates of error depend upon the error of y, which is estimated by $s^2$ (12.01) and are

$$V(b_1) = c_{11}s^2$$
$$V(b_2) = c_{22}s^2$$

where $c_{11}$ and $c_{22}$ are from the inverse matrix.

If $s^2$ is a valid estimate of the errors of the y's, then $c_{11}s^2$ and $c_{22}s^2$ will be valid estimates of the regression coefficients; no additional assumptions are required.

The error of $Y$ is an error of prediction. Its variance is given in (11.12). Note that while we assume that the error of y (obtained by actual measurement) is the same for all values of y, the error of $Y$ (calculated value) is least when $Y = \bar{y}$. In the neighborhood of $\bar{y}$ our calculated values are more reliable than those obtained by direct measurement. This outcome will appear natural enough if we reflect that by drawing the "best" line through our sequence of points we try, as it were, to adjust each point by considering its neighbors. Elementary algebra shows that the error of prediction and the error of direct measurement are equal when

$$x_0^2 = \frac{Sx^2(n - 1)}{n}$$

For values of x outside these limits the error of prediction is greater than the error of direct measurement.

13. Tests of Significance

Student's t-test is appropriate to most problems in least squares work. All forms of this test boil down to dividing a difference by its own (estimated) standard error. The test most frequently called for is directed at the regression coefficients.

Our coefficients $b_1$ and $b_2$ are assumed to be estimates of the unknown true values $\beta_1$ and $\beta_2$. Now, there may be some special values of the betas that we think particularly worthy of investigation. Most often of interest are the possibilities that one or both of the betas may be equal to zero. To say that $\beta_1$ is 0 is to say that the true line of regression passes through the origin. To say that $\beta_2$ is 0 is to say that the true line of regression is horizontal -- that is, that y and X are really independent.
To test, then, whether \( b_1 \) is different from zero we merely calculate

\[
t = \frac{b_1}{\text{S.E.}(b_1)}
\]

the standard error being of course the square root of the variance \( c_{11}s^2 \). If \( t \) exceeds the tabulated value at the desired significance level and for the number of D. F., we say that the coefficient \( b_1 \) is significant at the indicated level. So also for \( b_2 \), the division being of course by S. E. (\( b_2 \)), obtained by taking the square root of the variance \( c_{22}s^2 \).

13.01 Example: Test whether the coefficients found in (7.1.05) differ significantly from zero.

The equation is \( Y = 15 - 8 \); thus \( b_1 = 15, b_2 = 8 \). From (8.04) we have \( s^2 = 53.6 \). The matrix, from (7.1.03), is

\[
\begin{bmatrix}
7 & 21 \\
21 & 91 \\
\end{bmatrix}
\]

and the inverse or \( c \)-matrix is easily found; it is

\[
\begin{bmatrix}
13/28 & -3/28 \\
-3/28 & 1/28 \\
\end{bmatrix}
\]

Thus \( c_{11} = 13/28 \) and \( c_{22} = 1/28 \). We have then

\[
V(b_1) = c_{11}s^2 = 29.53 \quad \text{S. E. (}b_1\text{) = }5.43
\]

\[
V(b_2) = c_{22}s^2 = 2.27 \quad \text{S. E. (}b_2\text{) = }1.51
\]

To test whether the true value of \( b_1 \) is some hypothetical value \( b_0 \) we divide the difference by the standard error of \( b_1 \); if our hypothetical value is 0 we have simply

\[
t = \frac{b_1}{5.43} = \frac{15}{5.43} = 2.76 \quad \text{(5 D. F.)}
\]

Referring to a table of \( t \), we find that for 5 D. F. \( t > 2.57 \) has a probability of .05, and the probability for a larger value is of course smaller. Our result is thus significant at the 5\% level, and we can say with moderate confidence that our straight line does not pass through the origin.

Upon reflection, this result may seem somewhat academic. Even a casual look at the \( y \) column of (7.1.02) would probably convince us that the first value = +21 is not a random deviation from zero. There is in fact a suggestion that the bottle filling machine was deliberately set to overfill slightly at the beginning of the period, with some intention that early overfills would be compensated by later underfills. We should then expect zero deviation, not at the start of the period, but at the middle, corresponding to \( X_2 \) = 3 in (7.1.02). The observed value of \( y \) here is -11, the calculated value \( Y = -9 \), and applying the result of (11.12) we find the variance of \( Y = 9.09, \text{ S. E.} = 3.01 \). If \( Y = -9 \) is a chance fluctuation from a true value 0, it is a fluctuation of nearly 3 standard deviations, for \( t = -9/3.01 = 2.99 \) (still 5 D.F.) and again is significant at the 5\% level. We may thus say with some confidence that if it was the intention of the operator to set the machine in such a way that it would be delivering exactly the right volume at mid-period, his aim was a bit low.
To test whether the true value of $b_2$ might be zero we calculate
\[ t = \frac{b_2}{1.51} = 5.3, \]
which is significant for 5 D. F. at the 1% level. Here again our test is more academic than otherwise, since it would never occur to anyone, glancing at the data, that there is zero trend.

A more realistic test might be whether the trend exceeds some assigned value. Previous experience with the bottle filling machine may have taught us to expect a trend of (say) 10 units per hour, or 5 units per half-hour. The calculated value of $b_2$ is 8, meaning a trend of 8 units per half-hour. Is the observed trend significantly different from that expected from experience? The difference is $8 - 5 = 3$, not quite double the standard deviation of $b_2$; we therefore conclude that the difference is not significant. In other words, for all the data the true trend of the machine may be 5, and the calculated 8 may be merely a sampling variation. We can in fact calculate fiducial limits for $b_2$, which will be the largest and smallest values that give us a significant difference. For the 5% level we must have a difference of 2.57 standard deviations, or 3.88 (= 2.57 times 1.51) for significance; our 5% fiducial limits are thus $8 + 3.88 = 11.88$ and 11.88. Any hypothetical value for $b_2$ within these limits is consistent with the data, in the sense that the difference will not be significant at the 5% level. Of course, the "best" estimate in the maximum likelihood sense is the calculated value 8.

Another test that might be desired is on the end-point. We might be willing to run the machine to a moderate underfill, but wish to stop before the underfill became excessive. If we regard -25 as the limit of acceptable underfilling, we may ask "Had we run past the acceptable point at 11:30, when we had $y$ observed = -31, $Y$ calculated = -33? Either this -31 means we have overshot our mark, or it is a mere random fluctuation from -25, our desired limit. The difference is -8, and the standard error of $Y$, from (11.12), is
\[ \text{E. E. (} Y \text{)} = \sqrt{\frac{63.6(28 + 63)}{196}} = 5.43; \]
note that we have used $x$ in place of $X$ to obtain this. For our significance test we get $t = -8/5.43$, less than 2, and thus not significant at the 5% level. There is thus no proof in the data that we have run past our limit. It may be as well to mention, however, that if we are to control the consumer's as well as the producer's risk here, we shall need a more powerful method. A relevant discussion is given in Peach "Industrial Statistics and Quality Control", Section 30.2, which deals with "Variables Inspection: Double Limit on Mean".

It is sometimes of interest to draw, on either side of our least squares line, confidence bands giving the fiducial limits for $Y$ at each point on the line. The points on the curves which indicate the confidence bands are obtained by adding and subtracting to and from $Y$ the appropriate multiple of its standard error. Thus, for 5 D. F. and a 95% confidence band, we should calculate two curves:
\[ Y + 2.57 \text{ E. E. (} Y \text{)} \quad Y - 2.57 \text{ E. E. (} Y \text{)} . \]
These will be the two branches of a hyperbola. The line $Y = b_1 + b_2 X$ will be its conjugate axis. The distance between the two branches will be least for $\bar{y}$, since this is the value of $Y$ that has the smallest standard error. A complete investigation of the properties of this hyperbola would take us too far afield, but the student who is interested may do so with only elementary mathematics.
Analysis of Variance: Single Classification with Equal Subgroups

Suppose we are investigating a chemical process in which the yield is in some way dependent upon the pH (acid or basic reaction). We may know from earlier experiments that best results are obtained around pH 5; we wish now to pin the optimum pH down still closer. To this end we shall carry out a series of experiments, operating at pH 4.8, 5.0 and 5.4; we shall carry out five experiments at each pH, making 15 in all. Our problem is to measure the effect due to pH, and also to obtain an estimate of the experimental error so we can test the significance of differences. Our data will take the following form:

\[(14.01) \quad \text{pH} = 4.8 \quad \text{Yields:} \quad y_{11} \quad y_{12} \quad y_{13} \quad y_{14} \quad y_{15} \quad \text{Total} = R_1 \quad \text{Mean} \quad y_1.\]
\[5.0 \quad y_{21} \quad y_{22} \quad y_{23} \quad y_{24} \quad y_{25} \quad \text{R}_2 \quad y_2.\]
\[5.4 \quad y_{31} \quad y_{32} \quad y_{33} \quad y_{34} \quad y_{35} \quad \text{R}_3 \quad y_3.\]

Grand total \(S_y\) \quad Mean \(\bar{y}\).

Here \(R_k\) is the total for the first row and \(y_k\) (read \(y\)-one-dot) the mean of the first row = \(R_k / 5\). The total of all the \(y\)'s is \(S_y\), and the overall mean \(\bar{y}\).

How shall we proceed? We could of course fit a straight line, taking 4.8, 5.0 and 5.4 as our \(X\) values and \(R_1\), \(R_2\), and \(R_3\) as the \(y\)'s. One difficulty is that since we have data for only three values of \(X\), our line will be rather poorly defined. Moreover, our relationship may not be linear at all; indeed, the fact that we have chosen \(pH = 5.0\) as a sort of central value suggests that we rather expect a maximum or minimum nearby. While fitting a straight line to these data may be an interesting and profitable exercise, there exists a closely related technique called analysis of Variance, which leads to very simple computations and often useful results. It is this technique that we now introduce.

We need first to define the expression "The effect of Treatment A at the first (or second, or ...) level." In our example Treatment A consists of controlling the pH, and we do this at three levels: 4.8, 5.0, and 5.4. We may call these the first, second and third levels in any order that seems sensible. Suppose we call pH 4.8 the first level. Presumably working at this pH has some effect upon the average yield; maybe it tends to diminish it slightly. If working at pH 4.8 produces an average loss in yield of 3 units, we say the effect of Treatment A at the first level is minus 3. This would be the case, for instance, if the normal yield were 88 pounds but working at pH 4.8 gave an average yield of only 85 pounds. We shall usually think of an effect as being to raise (or lower) the average.

Now let us adopt the following notation:

\[b_1 = \text{average yield,}\]
\[b_2 = \text{effect of Treatment A at 1st level,}\]
\[b_3 = \text{ditto at 2nd level,}\]
\[b_4 = \text{ditto at 3rd level,}\]
\[e_{ij} = \text{experimental error of } y_{ij}.\]

Assume that each yield \(y_{ij}\) can be expressed as the sum of three components:

\[(14.02) \quad b_1, \quad \text{the average yield,}\]
\[b_2 \text{ or } b_3 \text{ or } b_4, \quad \text{the applicable treatment effect,}\]
\[e_{ij}, \quad \text{the error}.\]
We may then write

\[ Y_{ij} = b_1 X_1 + b_2 X_2 + b_3 X_3 + b_4 X_4 + e_{ij} \]

where \( X_1 \) is always \( 1 \) and one of the remaining \( x \)'s is unity, the other two being \( 0 \). Thus, \( y_{11} \) contains the overall mean, the first level effect, and the error; it does not contain the second and third level effects, so we may write these effects with coefficient zero, and the entire equation

\[ y_{11} = (1) b_1 + (1) b_2 + (0) b_3 + (0) b_4 + e_{11} \]

Leaving out terms with zero coefficients and omitting the one's, we shall have

(14.03)

\[
\begin{align*}
11 & = b_1 + b_2 \quad + e_{11} \\
12 & = b_1 + b_2 \quad + e_{12} \\
\vdots \\
15 & = b_1 + b_2 \quad + e_{15} \\
21 & = b_1 + b_3 \quad + e_{21} \\
\vdots \\
25 & = b_1 + b_2 \quad + e_{25} \\
31 & = b_1 + b_4 \quad + e_{31} \\
\vdots \\
35 & = b_1 \quad + b_4 + e_{35} 
\end{align*}
\]

Taking the coefficients of the \( b \)'s as the \( X \)'s of a least squares solution, we may think of a set of observations on \( X_1, X_2, X_3, X_4, \) and \( y \), thus:

(14.04)

\[
\begin{array}{cccccc}
1 & 1 & 0 & 0 & 11 \\
1 & 0 & 0 & 0 & 12 \\
1 & 0 & 0 & 1 & 13 \\
1 & 0 & 0 & 0 & 14 \\
1 & 0 & 1 & 0 & 15 \\
1 & 0 & 1 & 0 & 21 \\
1 & 0 & 1 & 0 & 22 \\
1 & 0 & 1 & 0 & 23 \\
1 & 0 & 1 & 0 & 24 \\
1 & 0 & 1 & 0 & 25 \\
1 & 0 & 0 & 1 & 31 \\
1 & 0 & 0 & 1 & 32 \\
1 & 0 & 0 & 1 & 33 \\
1 & 0 & 0 & 1 & 34 \\
1 & 0 & 0 & 1 & 35 \\
\end{array}
\]

\[
\begin{align*}
15 b_1 & + 5 b_2 + 5 b_3 + 5 b_4 = Sy \\
5 b_1 & + 5 b_2 = R_1 \\
5 b_1 & + 5 b_2 = R_2 \\
5 b_1 & + 5 b_4 = R_3 
\end{align*}
\]

(14.05) (the normal equations).
We see immediately that the normal equations are not independent, since the first is equal to the sum of the last three. This means that the set of equations has no unique solution. To understand why this is so, let us look back to the equations of (14.03). Two of these are

\[ y_{11} = b_1 + b_2 + e_{11}, \quad y_{21} = b_1 + b_3 + e_{21}. \]

Now, suppose we have a complete set of b's satisfying the equations of (14.03), and let k be any constant. We could then write

\[ y_{11} = (b_1 + k) + (b_2 - k) + e_{11} \quad y_{21} = (b_1 + k) + (b_3 - k) + e_{21} \]

without disturbing the equalities; the expressions in parentheses would satisfy our equations as well as the original b's, and would in fact be an alternative set. We could generate an infinite set of b's merely by adding and subtracting arbitrary constants. The operation is essentially that of measuring the various effects from different origins. If we adopt some convention to locate the origin it should then become possible to solve our normal equations.

The origin most commonly selected is \( \bar{y} \), which is taken as the b_1 of (14.02). All the effects b_2, b_3 and b_4 will then be measured as deviations from the overall mean. The first normal equation then becomes

\[ 15 \bar{y} + 5(b_1 + b_2 + b_3) = Sy, \]

and since of course \( 15\bar{y} = Sy \), we have necessarily

\[ (14.07) \quad b_1 + b_2 + b_3 = 0. \]

Thus, though we adopted the convention "Let b_1 = \( \bar{y} \)" to remove the singularity of the normal equations, we might equally have said "Let us assume that the sum of the treatment effects is zero" and been led to the same result. When we come to problems involving more than one treatment it will be more convenient to impose conditions like (14.07) and therefore we shall begin at once to think in these terms.

Starting with (14.07), then, we solve first the first normal equation.

\[ 15 b_1 + 5(b_2 + b_2 + b_3) = 5y \]

therefore

\[ 15 b_1 = Sy, \quad b_1 = \frac{Sy}{15}. \]

The remaining normal equations are now solved readily; substituting \( \bar{y} \) for \( b_1 \):

\[ 5\bar{y} + 5b_2 = R_1, \quad 5\bar{y} + 5b_3 = R_2, \quad 5\bar{y} + 5b_4 = R_3 \]

\[ b_2 = \frac{R_1}{5} - \bar{y}, \quad b_3 = \frac{R_2}{5} - \bar{y}, \quad b_4 = \frac{R_3}{5} - \bar{y}. \]

We find at last that the least squares estimates of the various effects are simply the differences between the row means and the general mean.

14.1 Numerical Example

In an experiment to study the removal of suspended matter from sewage by flocculation three substances were used: crude ferric sulfate, chlorinated copperas, and alum. Residual turbidity was measured with a candle turbidimeter. Fifteen aliquots of sewage were used, five for each treatment. The turbidity readings are given in (14.1.01).
Curve Fitting and Analysis of Variance

(14.1.01) Fe. sulf. 65 50 55 75 50 Total 295 Mean 59
Chl. Cop. 60 55 65 50 50 280 56
Alum 75 85 80 70 75 385 77
Grand total 960 \( \bar{y} = 64 \)

From (14.08) we have at once

(14.1.02) Effect of ferric sulfate = 59 - 64 = -5,
Effect of chlorinated copperas = 56 - 64 = -8,
Effect of alum = 77 - 64 = +13.

These are of course the estimates we should have made using common sense only, without statistics. The fact that the least squares solution and the common sense answer to this problem are the same is a partial justification of the method of least squares, and may give us more confidence in using least squares when the common sense answer is not so easy to see.

14.2 Precision of Treatment Effects

In (14.1.02) we find the iron salts making a better showing than alum, with chlorinated copperas giving a slightly better result than ferric sulfate. The difference is not great (3 units) and measurements with a candle turbidimeter are not very precise at best. We may thus reasonably inquire into the reliability of the observed-differences.

Let us look back at the equations of (14.03), remembering that we shall assume

(14.2.01) \[ b_2 + b_3 + b_4 = 0 \]

or \[ b_4 = -b_2 - b_3. \]

Those equations involving \( b_4 \) can be rewritten if we like, so that in place of

\[ y_{31} = b_1 + b_4 + e_{31} \]

we shall have

\[ y_{31} = b_1 - b_2 - b_3 + e_{31}; \]

so also for \( y_{32} \ldots y_{35} \). The tabular presentation (14.04) now appears without \( b_4 \), the coefficients of \( b_4 \) in (14.04) becoming coefficients of \( b_2 \) and \( b_3 \), all = -1.

(14.2.02) \[
\begin{array}{cccc|c}
X_1 & X_2 & X_3 & y \\
1 & 1 & 0 & y_{11} \\
1 & 1 & 0 & y_{12} \\
1 & 1 & 0 & y_{13} \\
1 & 1 & 0 & y_{14} \\
1 & 1 & 0 & y_{15} \\
1 & 0 & 1 & y_{21} \\
1 & 0 & 1 & y_{22} \\
1 & 0 & 1 & y_{23} \\
1 & 0 & 1 & y_{24} \\
1 & 0 & 1 & y_{25} \\
1 & -1 & -1 & y_{31} \\
1 & -1 & -1 & y_{32} \\
1 & -1 & -1 & y_{33} \\
1 & -1 & -1 & y_{34} \\
1 & -1 & -1 & y_{35} \\
\end{array}
\]

\[
\begin{align*}
S_{X_1}^2 &= 15 & S_{X_1X_2} &= S_{X_1X_3} &= 0 \\
S_{X_1y} &= S_y \\
S_{X_2}^2 &= 10 & S_{X_2X_3} &= 5 & S_{X_3}^2 &= 10 \\
S_{X_2y} &= R_1 - R_3 & S_{X_3y} &= R_2 - R_3 \\
The normal equations: & \quad 15b_1 = S_y \\
& \quad 10b_2 + 5b_3 = R_1 - R_3 \\
& \quad 5b_2 + 10b_3 = R_2 - R_3
\end{align*}
\]
Curve Fitting and Analysis of Variance

The a-matrix and its inverse (which is easily calculated) are

$$\text{(14.2.03)} \quad \begin{array}{ccc}
15 & 0 & 0 \\
0 & 10 & 5 \\
0 & 5 & 10
\end{array} \quad \begin{array}{ccc}
1/15 & 0 & 0 \\
0 & 2/15 & -1/15 \\
0 & -1/15 & 2/15
\end{array}$$

and we can apply (9.06) to get our b's.

$$b_1 = \frac{1}{15} \bar{Y} = \bar{y}$$

$$b_2 = \frac{2}{15} (R_1 - R_2) - \frac{1}{15} (R_2 - R_3)$$

$$b_3 = \frac{4}{15} (R_1 - R_3) + \frac{2}{15} (R_2 - R_3).$$

We get the same $b_1$ as before, but $b_2$ and $b_3$ look different. But if we write

$$15 b_2 = 2(R_1 - R_2) - (R_2 - R_3)$$

$$= 2R_1 - 2R_2 - R_2 + R_3$$

$$= 3R_1 - R_1 - R_2 - R_3 = 3R_1 - \bar{Y}$$

$$b_2 = Y_1 - \bar{y}$$

we see that $b_2$ is the same as before, and so of course is $b_3$. We can get $b_4$ if we like by using (14.2.01).

We are now in a position to calculate variances for our b's. First we have

$$Sv^2 = \bar{Y}^2 - \bar{y}^2$$

$$- (y_1 - \bar{y})(R_1 - R_2) - (y_2 - \bar{y})(R_2 - R_3).$$

In order to simplify this, consider the sum of the last two terms,

$$\text{(14.2.04)} \quad (y_1 - \bar{y})(R_1 - R_3) + (y_2 - \bar{y})(R_2 - R_3).$$

Adding a term whose value is zero will not change this sum, so we may write

$$= y_1(R_1 - R_3) + (y_2 - \bar{y})(R_2 - R_3) + (y_3 - \bar{y})(R_3 - R_3)$$

$$= y_1 R_1 + y_2 R_2 + y_3 R_3 - \bar{y}(R_1 + R_2 + R_3) - R_3 (y_1 + y_2 + y_3 - 3\bar{y}).$$

The last term is of course zero, and we have thus for (14.2.04)

$$\text{(14.2.05)} \quad Y_1 R_1 + y_2 R_2 + y_3 R_3 - \bar{y} Sy$$

which can also be written

$$\text{(14.2.06)} \quad \frac{R_1^2 + R_2^2 + R_3^2}{3} - \bar{y} Sy.$$
We can apply this result to the numerical example of (11.1) where \( s^2 = 63500 \).

\[ s^2 = 63500 - (6h)(960) - (62700 - 61h00) = 770. \]

We had 15 measurements and fitted three constants \((b_1, b_2, \text{ and } b_3)\) which leaves us 12 d.f. For our estimate of \( V(y) \) we have then

\[ s^2 = \frac{770}{12} = 64.17 \]

and the variances of the \( b \)'s can be obtained as usual.

\[ V(b_1) = c_{ll}s^2 = \frac{64.17}{15} = 4.28 \]

\[ V(b_2) = c_{22}s^2 = \frac{(64.17)(2)}{15} = 9.56 = c_{33}s^2 = V(b_3). \]

From considerations of symmetry it must be clear than \( V(b_1) = V(b_2) = V(b_3) \), but the fact can be proved directly by using the summation theorem for correlated variates. Let us denote by \( CV(x, y) \) the covariance of \( x \) and \( y \) -- that is, the expected value of the product \((X - \bar{x})(Y - \bar{y})\). Now, just as the variance of \( b_1 \) is estimated by \( c_{11}s^2 \), so the covariance of \( b_1 \) and \( b_2 \) is estimated by \( c_{13}s^2 \). From our inverse matrix (11.2.03) we see that \( CV(b_2, b_3) = -1/15s^2 \). The fundamental theorem for the variance of a sum of correlated variates is

\[ (11.2.08) \quad V(x + y) = V(x) + V(y) + 2 CV(x, y) \]

and this gives us

\[ V(b_1) = V(-b_2 - b_3) = V(b_2) + V(b_3) + 2 CV(b_2, b_3) = s^2(2/15). \]

We can use the same theorem to test the significance of the difference \( b_2 - b_3 \). In (11.1.02) this difference is only 3 units; does this justify us in saying that chlorinated copperas is more effective than ferric sulfate?

\[ V(b_2 - b_3) = V(b_2) + V(b_3) - 2 CV(b_2, b_3) = s^2(6/15) = 25.67. \]

\[ s. \quad (b_2 - b_3) = 5.07 \]

\[ t = \frac{3}{5.07} = .592 \quad (12 \text{ d. f.}) \]

which is of course not significant.

It should be easy to see that the difference \((b_2 - b_3)\) has the same standard error, and we have

\[ t = \frac{18}{5.07} = 3.55 \quad (12 \text{ d. f.}) \]

significant at the 1% level.

There is an important logical objection to the procedure we have just followed. The difference \((b_2 - b_1)\) is a function only of \( b_2 \) and \( b_3 \), and is correlated with \((b_2 - b_3)\). Only one of our t-tests is thus a random drawing from an unknown universe; the second t-test is partially determined by the outcome of the first. It is as if we were drawing cards from a very sticky pack, where drawing any card might result in bringing one of its neighbors with it; the idea of consecutive random drawings is not realized. To be sure, there are times when we have no better alternative than to accept some degree of dependence among our statistics; but in the present case we have an alternative procedure which has many merits.
14.3 Tests of Significance on Orthogonal Functions

Consider the functions

\[ Z_1 = a_{11}X_1 + a_{12}X_2 \quad Z_2 = a_{21}X_1 + a_{22}X_2 \]

where \( X_1 \) and \( X_2 \) are any random variables, possibly correlated. The covariance of \( Z_1 \) and \( Z_2 \) is by definition

\[ \text{CV}(Z_1, Z_2) = E(Z_1Z_2) - (EZ_1)(EZ_2) \]

which after a little algebra becomes

\[ \text{CV}(Z_1, Z_2) = a_{11}a_{21}V(X_1) + a_{12}a_{22}V(X_2) + (a_{11}a_{22} + a_{12}a_{21})(EX_1X_2 - EX_1EX_2). \]

This covariance will be zero if the following conditions are met:

\[ a_{11}a_{21} + a_{12}a_{22} = 0 \quad \text{i.e., both } X_1 \text{'s have the same variance} \]

\[ a_{11}a_{22} + a_{12}a_{21} = 0 \quad \text{the basic condition for orthogonality} \]

\[ (a_{11}a_{22} + a_{12}a_{21})(EX_1X_2 - EX_1EX_2) = 0 \quad \text{which assures the vanishing of } EX_1X_2. \]

As a special illustration of this theorem, consider the sum and difference of any two random variables:

\[ Z_1 = X_1 + X_2 \quad Z_2 = X_1 - X_2. \]

The theorem tells us that no matter what may be the correlation of \( X_1 \) and \( X_2 \), the \( Z_1 \)'s defined by these equations will be independent in the probability sense. We can if we like write \( Z_1 = k(X_1 + X_2) \) without loss of independence.

Now consider the quantity

\[ Z_1 = b_2 - b_3 \]

for which we have already obtained a significance test. The \( b_1 \)'s are of course correlated; but by (14.3.01) we can have also

\[ Z_2 = k(b_2 + b_3) \]

and \( Z_1 \) and \( Z_2 \) will be independent. Let \( k = -\frac{3}{2} \). Then

\[ Z_2 = -\frac{3}{2}(b_2 + b_3) = -(b_2 + b_3) - \frac{3}{2}(b_2 + b_3) = b_4 - \frac{3}{2}(b_2 + b_3). \]

Testing whether \( Z_1 \) is significantly different from zero is the same as testing the difference \( (b_2 - b_3) \). Testing whether \( Z_2 \) is significantly different from zero is the same as testing whether \( b_4 \) is significantly different from the mean of the other two \( b_1 \)'s \((b_2 + b_3)\) with which we would like to compare it. Since the tests are independent, we need have no fear that the result of one test has been biased by the other.

In our numerical example, this test is most appropriate. Our experiment used two iron salts and alum. It is natural to ask whether the iron salts were equally effective. On the face of it we should expect them to be so, and the data confirm our guess, since the difference \( (b_2 - b_3) \) is not significant. This being so, the alum result is naturally compared, not with one or the other of the iron results, but with the average of the two.