## 2. LEAST SQUARES ADJUSTMENT OF INDIRECT OBSERVATIONS

### 2.1. Introduction

The modern professional surveyor must be competent in all aspects of surveying measurements such as height differences, linear distances, horizontal and vertical angle measurements and combinations thereof which form the fundamental observations used to determine position in space. To obtain these measurements with any degree of confidence the surveyor must be aware of the principles and operation of various pieces of surveying equipment as well as the nature of measurements and the possible effects of errors on these measurements and any derived quantities. The nature of errors in measurements, studied by Gauss and leading to his theory of errors (the normal law of error) is the basis of statistical rules and tests that the surveyor employs to assess the quality of measurements; these rules and tests are covered in basic statistics courses during the undergraduate degree program. In the simple least squares processes and applications which follow it is sufficient to assume that the measurements are affected by small accidental or random errors and the least squares "solutions" provide a means of determining the best estimate of a measured quantity. Least squares solutions also imply that the quantity of interest has been determined from a redundant system of measurements, i.e., there are more measurements than the minimum number required to calculate the quantity.

### 2.1.1. Definition and classification of measurements

Crandall and Seabloom (1970, pp. 4-5) give a definition of a measurement as:

> A measurement is a comparison between an unknown quantity and a predefined standard, determined by some measuring device and hence, any measured value is an approximation of the exact or true value, not the true value itself. Since the true value of a quantity cannot be measured, any measurement contains by definition, an error.

Direct measurements (or observations) are those that are made directly upon the quantity to be determined. Measurements of a line by direct chaining, or Electronic Distance Measurement (EDM), or measurement of an angle by theodolite or Total Station are examples of direct measurements.

Indirect measurements (or observations) are not made upon the quantity itself but are made on some other quantity or quantities related to it. For example, the coordinates of a point $P$ are indirectly determined by measuring bearings and distances to $P$ from other points; the latitude of $P$ may be determined from altitudes to certain stars; and the height of $P$ may be determined by measured height differences from a known point.

### 2.1.2. Classification of errors of measurement

Since, by definition, every measurement contains an error it is necessary to consider the various kinds of errors that occur in practice. Rainsford (1968, p. 1) provides a derivation of the word error as:
coming from the Latin errare which means to wander and not to sin.

Rainsford divides errors into four classes
(a) blunders or mistakes
(b) constant errors
(c) systematic errors
(d) accidental or random errors

Blunders or mistakes are definite mis-readings, booking errors or other like occurrences.
They are usually caused by poor measurement technique and/or a lack of attention to detail by the person making the measurement. They may be eliminated or minimized by correct and careful measurement techniques, and a thorough understanding of the operation of the equipment used for the measurement.

Constant errors are those that do not vary throughout the particular measurement period. They are always of the same sign. Neglecting to standardize a measuring tape introduces a constant error; failure to use the correct prism-offset value introduces constant errors in EDM measurements. A faulty joint between sections of a levelling staff will introduce a constant error into height differences from spirit levelling. Constant errors can be eliminated from measurements by a thorough understanding of the measurement process and the equipment used.

Systematic errors are those errors that follow some fixed law (possibly unknown) dependent on local conditions and/or the equipment being used. For example, if the temperature and pressure (which are indicators of atmospheric conditions) are not measured when using EDM equipment then a systematic error may be introduced, since the modulated electromagnetic beam of the EDM passes through the atmosphere and its time of travel (indirectly measured by phase comparison of emitted and reflected beams) is affected by atmospheric conditions. All EDM measurements must be corrected for atmospheric conditions that depart from "standard conditions".

Accidental or Random errors are the small errors remaining in a measurement after mistakes, constant errors and systematic errors have been eliminated. They are due to the imperfection of the instruments used, the fallibility of the observer and the changing environmental conditions in which the measurements are made, all of which affect the measurement to a lesser or greater degree.

Bearing in mind the aforementioned, it could be said that all careful measurements (where mistakes, constant errors and systematic errors have been eliminated) contain small random errors and from experience, three axioms relating to random errors can be stated.

1. Small errors occur more frequently, or are more probable then large errors.
2. Positive and negative errors of the same magnitude are equally probable
3. Very large errors do not occur.

These axioms are the basic premises on which the theory of errors (the normal law of error) is founded.

### 2.1.3. Errors, corrections and residuals

A measured quantity has a true value and a most probable value. The most probable value is often called the best estimate and the two terms can be taken as synonymous.

No matter how many times a quantity is measured, its true value will remain unknown and only a best estimate can be obtained from the measurements. In the case of a single measured quantity, the best estimate is the arithmetic mean (or average) of the measurements.

If a quantity has been measured a number of times, the difference between the true (but unknown) value and any measurement is the true error and the difference between the best estimate and any measurement is the apparent error.

These relationships can be established by defining a correction to have the same magnitude as an error but the opposite sign. In surveying, the terms correction and residual are regarded as synonymous, and are universally denoted by the letter $v$.

Suppose an unknown quantity $x$ is measured $n$ times giving values $x_{1}, x_{2}, x_{3}, \ldots, x_{n}$. The true value (unknown) of the measured quantity is $\mu$ (mu) and is estimated by the arithmetic mean $\bar{X}$ where

$$
\begin{equation*}
\bar{x}=\frac{x_{1}+x_{2}+\cdots+x_{n}}{n}=\frac{\sum_{k=1}^{n} x_{k}}{n} \tag{2.1}
\end{equation*}
$$

The arithmetic mean is regarded as the best estimate or most probable value. A correction $v$ having the same magnitude as an error but the opposite sign is defined as

$$
v_{k}=\bar{x}-x_{k}
$$

Since these corrections relate to the measurements and arithmetic mean, they could be called apparent corrections and hence according to our definition of corrections and errors, apparent errors $-v$ are defined as

$$
-v_{k}=x_{k}-\bar{x}
$$

In a similar manner, we may define true errors $\varepsilon$ (epsilon) as

$$
\varepsilon_{k}=x_{k}-\mu
$$

These relationships may be expressed as

$$
\begin{aligned}
& \text { measurement }+ \text { residual } \quad=\text { best estimate } \\
& \text { measurement }- \text { best estimate }=\text { apparent error } \\
& \text { measurement }- \text { true value } \quad=\text { true error }
\end{aligned}
$$

True errors are unknown and are approximated by apparent errors. The closer the best estimate (or most probable value) approaches the true value, the closer the apparent error approaches the true error. The laws defining the nature and behaviour of true errors were derived from practical axioms deduced from the nature of apparent errors and hence any theory of errors may also be regarded as a theory of corrections (or residuals) and the distinction between true errors and apparent errors is ignored for all practical purposes.

The following sections contain simple examples of least squares processes, the mean, the weighted mean, line of best fit (linear regression) and polynomial curve fitting. In each case, Gauss' least squares principle: "... the most probable system of values of the quantities ... will be that in which the sum of the squares of the differences between the actually observed and computed values multiplied by numbers that measure the degree of precision, is a minimum." will be employed to determine equations or systems of equations that may be regarded as least squares solutions to the problems. Furthermore, it is assumed that all measurements are free of mistakes, constant errors and systematic errors and "contain" only random errors and that the precision of the measurements is known a priori (Latin a priori from what is before). Solutions to some of the examples are provided as MATLAB script files (.m files).

### 2.2. The Mean

It is well known practice that when a single quantity is measured a number of times the arithmetic mean is taken as the best estimate of the measured quantity. Few people realise that when they adopt this practice they are employing Gauss' least squares principle.

Consider a series of measurements $x_{1}, x_{2}, x_{3}, \ldots, x_{n}$ of a quantity and denote the best estimate of this quantity as $p$. According to our general definition of measurements and corrections we may write: measurement + correction (or residual) $=$ best estimate or

$$
x_{1}+v_{1}=p, x_{2}+v_{2}=p, x_{3}+v_{3}=p, \cdots, x_{n}+v_{n}=p
$$

These equations can be rearranged as

$$
v_{1}=p-x_{1}, v_{2}=p-x_{2}, v_{3}=p-x_{3}, \cdots, v_{n}=p-x_{n}
$$

Now if all the measurements can be regarded as having equal precision we may state the least squares principle as

The best estimate $p$ is that value which makes the sum of the squares of the residuals a minimum.

We may define a least squares function $\varphi$ (phi) as

$$
\begin{align*}
& \varphi=\text { the sum of the squares of the residuals }=\sum_{k=1}^{n} v_{k}^{2}  \tag{2.2}\\
& \varphi=\sum_{k=1}^{n} v_{k}^{2}=\left(p-x_{1}\right)^{2}+\left(p-x_{2}\right)^{2}+\cdots+\left(p-x_{n}\right)^{2}
\end{align*}
$$

or

We say that $\varphi$ is a function of $p$, the single parameter or variable in this equation. The minimum value of the function (i.e. making the sum of squares of residuals a minimum) can be found by equating the derivative $\frac{d \varphi}{d p}$ to zero, i.e.,

$$
\varphi \text { is a minimum when } \frac{d \varphi}{d p}=0
$$

and

$$
\frac{d \varphi}{d p}=2\left(p-x_{1}\right)+2\left(p-x_{2}\right)+\cdots+2\left(p-x_{n}\right)=0
$$

Cancelling the 2's and rearranging gives the best estimate $p$ as the arithmetic mean.

$$
\begin{equation*}
p=\frac{x_{1}+x_{2}+x_{3}+\cdots+x_{n}}{n}=\frac{\sum_{k=1}^{n} x_{k}}{n} \tag{2.3}
\end{equation*}
$$

Hence, the arithmetic mean of a series of measurements is the best estimate according to Gauss' least squares principle.

### 2.3. The Weighted Mean

Before demonstrating that the weighted mean of a set of observations is the result of a least squares process, some discussion of the term weight and its connection with precision is required.

### 2.3.1. Measures of Precision of a Finite Population

In every least squares process it is assumed that the precision of measurements is known. The precision is a measure of the dispersion (or spread) of a number of measurements from their mean (or average) value. A common statistical measure of precision is the variance $\sigma^{2}$ and the positive square root of the variance is the standard deviation $\sigma$. Equations for the variance and standard deviation differ depending on whether the population of measurements is finite or infinite and a population is a potential set of quantities that we want to make inference about based on a sample from that population.

Following Deakin and Kildea (1999), consider a finite population, such as the examination marks $m_{k}$ of a group of $N$ students in a single subject. Since we have complete information about the population, i.e., its size is known, the mean $\mu$, the variance $\sigma^{2}$ and the standard deviation $\sigma$ of the finite population are

$$
\begin{gather*}
\mu=\frac{\sum_{k=1}^{N} m_{k}}{N}  \tag{2.4}\\
\sigma^{2}=\frac{\sum_{k=1}^{N}\left(m_{k}-\mu\right)^{2}}{N}  \tag{2.5}\\
\sigma=\sqrt{\frac{\sum_{k=1}^{N}\left(m_{k}-\mu\right)^{2}}{N}} \tag{2.6}
\end{gather*}
$$

Note that the variance $\sigma^{2}$ is the average squared difference of a member of the population $m_{k}$ from the population mean $\mu$. The mean, variance and standard deviation are known as population parameters.

### 2.3.2. Estimates of Precision of Samples of an Infinite Population

Consider surveying measurements, drawn from infinite populations with the attendant difficulties of estimation since population averages can never be known. In such cases we are usually dealing with small samples of measurements of size $n$ and we can only obtain estimates of the unknown population parameters $\mu, \sigma^{2}$ and $\sigma$. For a sample of $n$
measurements $x_{1}, x_{2}, x_{3}, \ldots, x_{n}$ from an infinite population, estimates of the mean, variance and standard deviation, denoted by $\bar{x}, s_{x}^{2}$ and $s_{x}$ are

$$
\begin{gather*}
\bar{x}=\frac{1}{n} \sum_{k=1}^{n} x_{k}  \tag{2.7}\\
s_{x}^{2}=\frac{1}{n-1} \sum_{k=1}^{n}\left(x_{k}-\bar{x}\right)^{2}  \tag{2.8}\\
s_{x}=\sqrt{\frac{1}{n-1} \sum_{k=1}^{n}\left(x_{k}-\bar{x}\right)^{2}} \tag{2.9}
\end{gather*}
$$

Note the divisor $n-1$ (known as the degrees of freedom) in equations for the estimates of variance and standard deviation. This ensures that $s_{x}^{2}$ is an unbiased estimate of the population variance $\sigma^{2}$, but does not ensure that $s_{x}$ is an unbiased estimate of the population standard deviation $\sigma$; the action of "taking a square-root" changes the property of unbiasedness. This is more an accident of mathematics rather than a cause of faulty estimation but it is not well appreciated in general. Deakin and Kildea (1999, p. 76) show that an unbiased estimator $s_{x}^{*}$ of the population standard deviation $\sigma$ is given by

$$
\begin{equation*}
s_{x}^{*}=\sqrt{\frac{1}{c_{n}} \sum_{k=1}^{n}\left(x_{k}-\bar{x}\right)^{2}} \tag{2.10}
\end{equation*}
$$

Values of $c_{n}$ are given in Table 2.1

| $n$ | 2 | 3 | 4 | 5 | 10 | 15 | 20 | 30 | 90 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $n-1$ | 1 | 2 | 3 | 4 | 9 | 14 | 19 | 29 | 89 |
| $c_{n}$ | 0.64 | 1.57 | 2.55 | 3.53 | 8.51 | 13.51 | 18.51 | 28.50 | 88.50 |

Table 2.1 Values of divisor $c_{n}$ for unbiased estimation of $\sigma$

In these notes, it is always assumed that the terms mean, variance and standard deviation refer to estimates of population values.

### 2.3.3. Relationship between Weights and Estimates of Variance

Another measure of precision, often used in least squares applications is weight $w$ and the weight of an observation (or measurement) is defined as being inversely proportional to the variance

$$
\begin{align*}
& w_{k} \propto \frac{1}{s_{k}^{2}}  \tag{2.11}\\
& w_{k}=\frac{\sigma_{0}^{2}}{s_{k}^{2}} \tag{2.12}
\end{align*}
$$

$\sigma_{0}^{2}$ is a constant of proportionality known as the reference variance or variance factor. This is the classical definition of weight and if an observation has unit weight $\left(w_{k}=1\right)$ its variance equals $\sigma_{0}^{2}$, hence the reference variance is sometimes called the variance of an observation of unit weight; a term often encountered in older surveying texts. In this definition of weight, there is an assumption that the measurements are uncorrelated (a statistical term relating to the dependence between measurements, see section 2.5). In cases where measurements are correlated, weights are not an adequate means of describing relative precisions.

As an example of the connection between weights and standard deviations consider three uncorrelated (i.e., independent) observations of a particular distance, where each observation is the mean of several measurements and standard deviations of each observation have been determined from the measurements
observation $1 \quad 136.225 \mathrm{~m}$ (st. dev. 0.010 m )
observation $2 \quad 136.233 \mathrm{~m}$ (st. dev. 0.032 m )
observation $3 \quad 136.218 \mathrm{~m}$ (st. dev. 0.024 m )

Since the weight is inversely proportional to the variance, the observation with the smallest weight will have the largest variance (standard deviation squared). For convenience, this observation is given unit weight i.e., $w_{2}=1$ and the other observations (with smaller variances) will have higher weight. Hence from (2.12)

$$
w_{2}=1=\frac{\sigma_{0}^{2}}{(0.032)^{2}} \quad \text { and } \quad \sigma_{0}^{2}=(0.032)^{2}
$$

The weights of the three observations are then

$$
\begin{aligned}
& w_{1}=\frac{(0.032)^{2}}{(0.010)^{2}}=10.24 \\
& w_{2}=\frac{(0.032)^{2}}{(0.032)^{2}}=1 \\
& w_{3}=\frac{(0.032)^{2}}{(0.024)^{2}}=1.78
\end{aligned}
$$

Weights are often assigned to observations using "other information". Say for example, a distance is measured three times and a mean value determined. If two other determinations of the distance are from the means of six and four measurements respectively, the weights of the three observations may simply be assigned the values 3,6 and 4 . This assignment of weights is a very crude reflection of the (likely) relative precisions of the observations since it is known that to double the precision of a mean of a set of measurements, we must quadruple the number of measurements taken (Deakin and Kildea, 1999, p. 76).

### 2.3.4. Derivation of Equation for the Weighted Mean

Consider a set of measurements of a quantity as $x_{1}, x_{2}, x_{3}, \ldots, x_{n}$ each having weight $w_{1}, w_{2}, w_{3}, \ldots, w_{n}$ and denote the best estimate of this quantity as $q$. According to our general definition of measurements and corrections we may write:
measurement + correction (or residual) = best estimate
or

$$
x_{1}+v_{1}=q, x_{2}+v_{2}=q, x_{3}+v_{3}=q, \cdots, x_{n}+v_{n}=q
$$

These equations can be rearranged as

$$
v_{1}=q-x_{1}, v_{2}=q-x_{2}, v_{3}=q-x_{3}, \cdots, v_{n}=q-x_{n}
$$

Now each measurement has a weight reflecting relative precision and we may state the least squares principle as

The best estimate $q$ is that value which makes the sum of the squares of the residuals, multiplied by their weights, a minimum.
We may define a least squares function $\varphi$ (phi) as

$$
\begin{equation*}
\varphi=\text { the sum of the weighted squared residuals }=\sum_{k=1}^{n} w_{k} v_{k}^{2} \tag{2.13}
\end{equation*}
$$

or

$$
\varphi=\sum_{k=1}^{n} w_{k} v_{k}^{2}=w_{1}\left(q-x_{1}\right)^{2}+w_{2}\left(q-x_{2}\right)^{2}+\cdots+w_{n}\left(q-x_{n}\right)^{2}
$$

We say that $\varphi$ is a function of $q$, the single parameter or variable in this equation. The minimum value of the function (i.e., making the sum of the weighted squared residuals a minimum) can be found by equating the derivative $\frac{d \varphi}{d q}$ to zero, i.e.,

$$
\varphi \text { is a minimum when } \frac{d \varphi}{d q}=0
$$

and

$$
\frac{d \varphi}{d q}=2 w_{1}\left(q-x_{1}\right)+2 w_{2}\left(q-x_{2}\right)+\cdots+2 w_{n}\left(q-x_{n}\right)=0
$$

Cancelling the 2's and expanding gives

$$
w_{1} q-w_{1} x_{1}+w_{2} q-w_{2} x_{2}+\cdots+w_{n} q-w_{n} x_{n}=0
$$

Rearranging gives the weighted arithmetic mean $q$

$$
\begin{equation*}
q=\frac{w_{1} x_{1}+w_{2} x_{2}+\cdots+w_{n} x_{n}}{w_{1}+w_{2}+\cdots+w_{n}}=\frac{\sum_{k=1}^{n} w_{k} x_{k}}{\sum_{k=1}^{n} w_{k}} \tag{2.14}
\end{equation*}
$$

Hence, the weighted arithmetic mean of a series of measurements $x_{k}$ each having weight $w_{k}$ is the best estimate according to Gauss' least squares principle.

It should be noted that the equation for the weighted mean (2.14) is valid only for measurements that are statistically independent. If observations are dependent, then a measure of the dependence between the measurements, known as covariance, must be taken into account. A more detailed discussion of weights, variances and covariances is given in later sections of these notes.

### 2.4. Line of Best Fit



Figure 2.1 Line of Best Fit through data points 1 to 5

The line of best fit shown in the Figure 2.1 has the equation $y=m x+c$ where $m$ is the slope of the line $\left(m=\tan \theta=\frac{y_{2}-y_{1}}{x_{2}-x_{1}}\right)$ and $c$ is the intercept of the line on the $y$ axis.
$m$ and $c$ are the parameters and the data points are assumed to accord with the mathematical model $y=m x+c$. Obviously, only two points are required to define a straight line and so three of the five points in Figure 2.1 are redundant measurements (or observations). In this example the $x, y$ coordinate pairs of each data point are considered as indirect measurements of the parameters $m$ and $c$ of the mathematical model.

To estimate (or compute) values for $m$ and $c$, pairs of points in all combinations (ten in all) could be used to obtain average values of the parameters; or perhaps just two points selected as representative could be used to determine $m$ and $c$.

A better way is to determine a line such that it passes as close as possible to all the data points. Such a line is known as a Line of Best Fit and is obtained (visually) by minimising the differences between the line and the data points. No account is made of the "sign" of these differences, which can be considered as corrections to the measurements or residuals. The Line of Best Fit could also be defined as the result of a least squares process that determines estimates of the parameters $m$ and $c$ such that those values will make the sum of the squares of the residuals, multiplied by their weights, a minimum. Two examples will be considered, the first with all measurements considered as having equal precisions, i.e., all weights of equal value, and the second, measurements having different precisions, i.e., unequal weights.

### 2.4.1. Line of Best Fit (equal weights)

In Figure 2.1 there are five data points whose $x, y$ coordinates (scaled from the diagram in mm's) are

| Point | $x$ | $y$ |
| :---: | :---: | :---: |
| 1 | -40.0 | -24.0 |
| 2 | -15.0 | -24.0 |
| 3 | 10.0 | -12.0 |
| 4 | 38.0 | 15.0 |
| 5 | 67.0 | 30.0 |

Table 2.2 Coordinates of data points (mm's) shown in Figure 2.1

Assume that the data points accord with the mathematical model $y=m x+c$ and each measurement has equal precision. Furthermore, assume that the residuals are associated with the $y$ values only, which leads to an observation equation of the form

$$
\begin{equation*}
y_{k}+v_{k}=m x_{k}+c \tag{2.15}
\end{equation*}
$$

By adopting this observation equation we are actually saying that the measurements (the $x, y$ coordinates) don't exactly fit the mathematical model, i.e., there are inconsistencies between the model and the actual measurements, and these inconsistencies (in both $x$ and $y$ measurements) are grouped together as residuals $v_{k}$ and simply added to the left-hand-side of the mathematical model. This is simply a convenience. We could write an observation equation of the form

$$
y_{k}+v_{y_{k}}=m\left(x_{k}+v_{x_{k}}\right)+c
$$

$v_{x_{k}}, v_{y_{k}}$ are residuals associated with the $x$ and $y$ coordinates of the $k^{\text {th }}$ point. Observation equations of this form require more complicated least squares solutions and are not considered in this elementary section.

Equations (2.15) can be re-written as residual equations of the form

$$
\begin{equation*}
v_{k}=m x_{k}+c-y_{k} \tag{2.16}
\end{equation*}
$$

The distinction here between observation equations and residual equations is simply that residual equations have only residuals on the left of the equals sign. Rearranging observation equations into residual equations is an interim step to simplify the function $\varphi=$ sum of squares of residuals.

Since all observations are of equal precision (equal weights), the least squares function to be minimised is

$$
\varphi=\text { the sum of the squares of the residuals }=\sum_{k=1}^{n} v_{k}^{2}
$$

or

$$
\varphi=\sum_{k=1}^{5} v_{k}^{2}=\left(m x_{1}+c-y_{1}\right)^{2}+\left(m x_{2}+c-y_{2}\right)^{2}+\ldots .+\left(m x_{5}+c-y_{5}\right)^{2}
$$

$\varphi$ is a function of the $u=2$ "unknown" parameters $m$ and $c$ and so to minimise the sum of squares of residuals, the partial derivatives $\frac{\partial \varphi}{\partial m}$ and $\frac{\partial \varphi}{\partial c}$ are equated to zero.

$$
\begin{aligned}
& \frac{\partial \phi}{\partial m}=2\left(m x_{1}+c-y_{1}\right)\left(x_{1}\right)+2\left(m x_{2}+c-y_{2}\right)\left(x_{2}\right)+\ldots+2\left(m x_{5}+c-y_{5}\right)\left(x_{5}\right)=0 \\
& \frac{\partial \phi}{\partial c}=2\left(m x_{1}+c-y_{1}\right)(1)+2\left(m x_{2}+c-y_{2}\right)(1)+\ldots+2\left(m x_{5}+c-y_{5}\right)(1)=0
\end{aligned}
$$

Cancelling the 2's, simplifying and re-arranging gives two normal equations of the form

$$
\begin{align*}
m \sum_{k=1}^{n} x_{k}^{2}+c \sum_{k=1}^{n} x_{k} & =\sum_{k=1}^{n} x_{k} y_{k} \\
m \sum_{k=1}^{n} x_{k}+c n & =\sum_{k=1}^{n} y_{k} \tag{2.17}
\end{align*}
$$

The normal equations can be expressed in matrix form as

$$
\begin{gather*}
{\left[\begin{array}{cc}
\sum x_{k}^{2} & \sum x_{k} \\
\sum x_{k} & n
\end{array}\right]\left[\begin{array}{l}
m \\
c
\end{array}\right]=\left[\begin{array}{l}
\sum x_{k} y_{k} \\
\sum y_{k}
\end{array}\right]}  \tag{2.18}\\
\mathbf{N} \mathbf{x}=\mathbf{t} \tag{2.19}
\end{gather*}
$$

Matrix algebra is a powerful mathematical tool that simplifies the theory associated with least squares. The student should become familiar with the terminology and proficient with the algebra. Appendix A contains useful information relating to matrix algebra.

$$
\begin{aligned}
& \mathbf{N}=\left[\begin{array}{ll}
n_{11} & n_{12} \\
n_{21} & n_{22}
\end{array}\right] \quad \text { is the }(u, u) \underline{\text { normal equation coefficient matrix }} \\
& \mathbf{x}=\left[\begin{array}{l}
x_{1} \\
x_{2}
\end{array}\right]
\end{aligned} \quad \text { is the }(u, 1) \text { vector of parameters (or "unknowns"), and } \quad \begin{array}{ll}
\mathbf{t}=\left[\begin{array}{l}
t_{1} \\
t_{2}
\end{array}\right] & \text { is the }(u, 1) \underline{\text { vector of numeric terms. }}
\end{array}
$$

The solution of the normal equations for the vector of parameters is

$$
\begin{equation*}
\mathbf{x}=\mathbf{N}^{-1} \mathbf{t} \tag{2.20}
\end{equation*}
$$

In this example (two equations in two unknowns) the matrix inverse $\mathbf{N}^{-1}$ is easily obtained (see Appendix A 4.8) and the solution of (2.20) is given as

$$
\mathbf{x}=\left[\begin{array}{l}
x_{1}  \tag{2.21}\\
x_{2}
\end{array}\right]=\frac{1}{\left(n_{11} n_{22}-n_{12} n_{21}\right)}\left[\begin{array}{cc}
n_{22} & -n_{12} \\
-n_{21} & n_{11}
\end{array}\right]\left[\begin{array}{l}
t_{1} \\
t_{2}
\end{array}\right]
$$

From the data given in Table 2.2, the normal equations are

$$
\left[\begin{array}{rr}
7858.00 & 60.00 \\
60.00 & 5.00
\end{array}\right]\left[\begin{array}{l}
m \\
c
\end{array}\right]=\left[\begin{array}{r}
3780.00 \\
-15.00
\end{array}\right]
$$

and the solutions for the best estimates of the parameters $m$ and $c$ are

$$
\left[\begin{array}{c}
m \\
c
\end{array}\right]=\frac{1}{(7858.00)(5.00)-(60.00)(60.00)}\left[\begin{array}{cc}
5.00 & -60.00 \\
-60.00 & 7858.00
\end{array}\right]=\left[\begin{array}{c}
0.554777 \\
-9.657327
\end{array}\right]
$$

Substitution of the best estimates of the parameters $m$ and $c$ into the residual equations $v_{k}=m x_{k}+c-y_{k}$ gives the residuals (mm's) as

$$
\begin{array}{rr}
v_{1}= & -7.8 \\
v_{2}= & 6.0 \\
v_{3}= & 7.9 \\
v_{4}= & -3.6 \\
v_{5}= & -2.5
\end{array}
$$

### 2.4.2. Line of Best Fit (unequal weights)

Consider again the Line of best Fit shown in Figure 2.1 but this time the $x, y$ coordinate pairs are weighted, i.e., some of the data points are considered to have more precise coordinates than others. Table 2.3 shows the $x, y$ coordinates (scaled from the diagram in mm's) with weights.

| Point | $x$ | $y$ | weight $w$ |
| :---: | :---: | :---: | :---: |
| 1 | -40.0 | -24.0 | 2 |
| 2 | -15.0 | -24.0 | 5 |
| 3 | 10.0 | -12.0 | 7 |
| 4 | 38.0 | 15.0 | 3 |
| 5 | 67.0 | 30.0 | 3 |

Table 2.3 Coordinates (mm) and weights of data points shown in Figure 2.1

Similarly to before, a residual equation of the form given by (2.16) can be written for each observation but this time a weight $w_{k}$ is associated with each equation and the least squares function to be minimised is

$$
\varphi=\text { the sum of the weighted squared residuals }=\sum_{k=1}^{n} w_{k} v_{k}^{2}
$$

or $\quad \varphi=\sum_{k=1}^{5} w_{k} v_{k}^{2}=w_{1}\left(m x_{1}+c-y_{1}\right)^{2}+w_{2}\left(m x_{2}+c-y_{2}\right)^{2}+\ldots .+w_{5}\left(m x_{5}+c-y_{5}\right)^{2}$
$\varphi$ is a function of the $u=2$ "unknown" parameters $m$ and $c$ and so to minimise $\varphi$ the partial derivatives $\frac{\partial \varphi}{\partial m}$ and $\frac{\partial \varphi}{\partial c}$ are equated to zero.

$$
\begin{aligned}
& \frac{\partial \phi}{\partial m}=2 w_{1}\left(m x_{1}+c-y_{1}\right)\left(x_{1}\right)+2 w_{2}\left(m x_{2}+c-y_{2}\right)\left(x_{2}\right)+\ldots+2 w_{5}\left(m x_{5}+c-y_{5}\right)\left(x_{5}\right)=0 \\
& \frac{\partial \phi}{\partial c}=2 w_{1}\left(m x_{1}+c-y_{1}\right)(1)+2 w_{2}\left(m x_{2}+c-y_{2}\right)(1)+\ldots+2 w_{5}\left(m x_{5}+c-y_{5}\right)(1)=0
\end{aligned}
$$

Cancelling the 2's simplifying and re-arranging gives two normal equations of the form

$$
\begin{aligned}
& m \sum_{k=1}^{n} w_{k} x_{k}^{2}+c \sum_{k=1}^{n} w_{k} x_{k}=\sum_{k=1}^{n} w_{k} x_{k} y_{k} \\
& m \sum_{k=1}^{n} w_{k} x_{k}+c \sum_{k=1}^{n} w_{k}=\sum_{k=1}^{n} w_{k} y_{k}
\end{aligned}
$$

The normal equations expressed in matrix form $\mathbf{N x}=\mathbf{t}$ are

$$
\left[\begin{array}{cc}
\sum w_{k} x_{k}^{2} & \sum w_{k} x_{k} \\
\sum w_{k} x_{k} & \sum w_{k}
\end{array}\right]\left[\begin{array}{l}
m \\
c
\end{array}\right]=\left[\begin{array}{l}
\sum w_{k} x_{k} y_{k} \\
\sum w_{k} y_{k}
\end{array}\right]
$$

Substituting the data in Table 2.3, the normal equations are

$$
\left[\begin{array}{rr}
22824.00 & 230.00 \\
230.00 & 20.00
\end{array}\right]\left[\begin{array}{l}
m \\
c
\end{array}\right]=\left[\begin{array}{r}
10620.00 \\
-117.00
\end{array}\right]
$$

The solution for the best estimates of the parameters $m$ and $c$ is found in exactly the same manner as before (see section 2.4.1)

$$
\begin{aligned}
& m=0.592968 \\
& c=-12.669131
\end{aligned}
$$

Substitution of $m$ and $c$ into the residual equations $v_{k}=m x_{k}+c-y_{k}$ gives the residuals (mm's) as

$$
\begin{array}{rr}
v_{1}= & -12.4 \\
v_{2}= & 2.4 \\
v_{3}= & 5.3 \\
v_{4}= & -5.1 \\
v_{5}= & -2.9
\end{array}
$$

Comparing these residuals with those from the Line of Best Fit (equal weights), shows that the line has been pulled closer to points 2 and 3, i.e.; the points having largest weight.

### 2.5. Variances, Covariances, Cofactors and Weights

Some of the information in this section has been introduced in previously in section 2.3 The Weighted Mean and is re-stated here in the context of developing general matrix expressions for variances, covariances, cofactors and weights of sets or arrays of measurements.

In surveying applications, we may regard a measurement $x$ as a possible value of a continuous random variable drawn from an infinite population. To model these populations, and thus estimate the quality of the measurements, probability density functions have been introduced. In surveying, Normal (Gaussian) probability density functions are the usual model. A probability density function is a non-negative function where the area under the curve is one. For $f(x) \geq 0$ and $\int_{-\infty}^{+\infty} f(x) d x=1$ the values of $f(x)$ are not probabilities. The probability a member of the population lies in the interval $a$ to $b$ is $\int_{a}^{b} f(x) d x$. The population mean $\mu$, population variance $\sigma_{x}^{2}$ and the family of Normal probability density functions are given by Kreyszig (1970) as

$$
\begin{gather*}
\mu_{x}=\int_{-\infty}^{+\infty} x f(x) d x  \tag{2.22}\\
\sigma_{x}^{2}=\int_{-\infty}^{+\infty}\left(x-\mu_{x}\right)^{2} f(x) d x  \tag{2.23}\\
f\left(x ; \mu_{x}, \sigma_{x}\right)=\frac{1}{\sigma_{x} \sqrt{2 \pi}} e^{-\frac{1}{2}\left(\frac{x-\mu_{x}}{\sigma_{x}}\right)^{2}} \tag{2.24}
\end{gather*}
$$

Since the population is infinite, means and variances are never known, but may be estimated from a sample of size $n$. The sample mean $\bar{x}$ and sample variance $s_{x}^{2}$, are unbiased estimates of the population mean $\mu_{x}$ and population variance $\sigma_{x}^{2}$

$$
\begin{gather*}
\bar{x}=\frac{1}{n} \sum_{k=1}^{n} x_{k}  \tag{2.25}\\
s_{x}^{2}=\frac{1}{n-1} \sum_{k=1}^{n}\left(x_{k}-\bar{x}\right)^{2} \tag{2.26}
\end{gather*}
$$

The sample standard deviation $s_{\chi}$ is the positive square root of the sample variance and is a measure of the precision (or dispersion) of the measurements about the mean $\bar{x}$.

In least squares applications, an observation may be the mean of a number measurements or a single measurement. In either case, it is assumed to be from an infinite population of measurements having a certain (population) standard deviation and that an estimate this standard deviation is known.

When two or more observations are jointly used in a least squares solution then the interdependence of these observations must be considered. Two measures of this interdependence are covariance and correlation. For two random variables $x$ and $y$ with a joint probability density function $f(x, y)$ the covariance $\sigma_{x y}$ is

$$
\begin{equation*}
\sigma_{x y}=\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty}\left(x-\mu_{x}\right)\left(y-\mu_{y}\right) f(x, y) d x d y \tag{2.27}
\end{equation*}
$$

and the correlation coefficient $\rho$ is given by

$$
\begin{equation*}
\rho_{x y}=\frac{\sigma_{x y}}{\sigma_{x} \sigma_{y}} \tag{2.28}
\end{equation*}
$$

The correlation coefficient $\rho$ will vary between $\pm 1$. If $\rho_{x y}=0$ random variables $x$ and $y$ are said to be uncorrelated and, if $\rho_{x y}= \pm 1, x$ and $y$ are linked by a linear relationship (Kreyszig 1970, pp.335-9). Correlation and statistical dependence are not the same, although both concepts are used synonymously. It can be shown that the covariance $\sigma_{x y}$ is always zero when the random variables are statistically independent (Kreyszig 1970, p.137-9). Unfortunately, the reverse is not true in general. Zero covariance does not necessarily imply statistical independence. Nevertheless, for multivariate Normal probability density functions, zero covariance (no correlation) is a sufficient condition for statistical independence (Mikhail 1976, p.19).

The sample covariance $s_{x y}$ between $n$ pairs of values $\left(x_{1}, y_{1}\right),\left(x_{2}, y_{2}\right), \ldots,\left(x_{n}, y_{n}\right)$ with means $\bar{x}$ and $\bar{y}$ is (Mikhail 1976, p.43)

$$
\begin{equation*}
s_{x y}=\frac{1}{n-1} \sum_{k=1}^{n}\left(x_{k}-\bar{x}\right)\left(y_{k}-\bar{y}\right) \tag{2.29}
\end{equation*}
$$

Variances and covariances of observations can be conveniently represented using matrices. For $n$ observations $x_{1}, x_{2}, x_{3}, \ldots, x_{n}$ with variances $\sigma_{1}^{2}, \sigma_{2}^{2}, \sigma_{3}^{2}, \ldots, \sigma_{n}^{2}$ and covariances $\sigma_{12}, \sigma_{13}, \ldots$ the variance-covariance matrix $\Sigma$ is defined as

$$
\Sigma=\left[\begin{array}{cccc}
\sigma_{1}^{2} & \sigma_{12} & \sigma_{13} & \ldots \sigma_{1 n}  \tag{2.30}\\
\sigma_{21} & \sigma_{2}^{2} & \sigma_{23} & \ldots \sigma_{2 n} \\
\ldots . & \ldots . & \ldots . & \ldots . \\
\sigma_{n 1} & \sigma_{n 2} & \sigma_{n 3} & \ldots \sigma_{n n}^{2}
\end{array}\right]
$$

Note that the variance-covariance matrix $\Sigma$ is symmetric since in general $\sigma_{k j}=\sigma_{j k}$.

In practical applications of least squares, population variances and covariances are unknown and are replaced by estimates $s_{1}^{2}, s_{2}^{2}, \ldots, s_{n}^{2}$ and $s_{12}, s_{13}, \ldots$ or by other numbers representing relative variances and covariances. These are known as cofactors and the cofactor matrix $\mathbf{Q}$, which is symmetric, is defined as

$$
\mathbf{Q}=\left[\begin{array}{cccc}
q_{11} & q_{12} & q_{13} & \ldots q_{1 n}  \tag{2.31}\\
q_{21} & q_{22} & q_{23} & \ldots q_{2 n} \\
\ldots . . & \ldots . & \ldots & \ldots . \\
q_{n 1} & q_{n 2} & q_{n 3} & \ldots q_{n n}
\end{array}\right]
$$

The relationship between variance-covariance matrices and cofactor matrices is

$$
\begin{equation*}
\Sigma=\sigma_{0}^{2} \mathbf{Q} \tag{2.32}
\end{equation*}
$$

$\sigma_{0}^{2}$ is a scalar quantity known as the variance factor. The variance factor is also known as the reference variance and the variance of an observation of unit weight (see section 2.3 for further discussion on this subject).

The inverse of the cofactor matrix $\mathbf{Q}$ is the weight matrix $\mathbf{W}$.

$$
\begin{equation*}
\mathbf{W}=\mathbf{Q}^{-1} \tag{2.33}
\end{equation*}
$$

Note that since $\mathbf{Q}$ is symmetric, its inverse $\mathbf{W}$ is also symmetric. In the case of uncorrelated observations, the variance-covariance matrix $\Sigma$ and the cofactor matrix $\mathbf{Q}$ are both diagonal matrices (see Appendix A) and the weight of an observation $w$ is a value that is inversely proportional to the estimate of the variance i.e.,

$$
\begin{equation*}
w_{k k}=\sigma_{0}^{2} / q_{k k} \quad \text { or } \quad w_{k k}=\sigma_{0}^{2} / s_{k k}^{2} \tag{2.34}
\end{equation*}
$$

For uncorrelated observations, the off-diagonal terms will be zero and the double subscripts may be replaced by single subscripts; equation (2.34) becomes

$$
\begin{equation*}
w_{k}=\sigma_{0}^{2} / s_{k}^{2} \tag{2.35}
\end{equation*}
$$

This is the classical definition of a weight where $\sigma_{0}^{2}$ is a constant of proportionality.

Note: The concept of weights has been extensively used in classical least squares theory but is limited in its definition to the case of independent (or uncorrelated) observations. (Mikhail 1976, pp.64-65 and Mikhail and Gracie 1981, pp.66-68).

### 2.6. Matrices and Simple Least Squares Problems

Matrix algebra is a powerful mathematical tool that can be employed to develop standard solutions to least squares problems. The previous examples of the Line of Best Fit will be used to show the development of standard matrix equations that can be used for any least squares solution.

In previous developments, we have used a least squares function $\varphi$ as meaning either the sum of squares of residuals or the sum of squares of residuals multiplied by weights.

In the Line of Best Fit (equal weights), we used the least squares function

$$
\varphi=\text { the sum of the squares of the residuals }=\sum_{k=1}^{n} v_{k}^{2}
$$

If the residuals $v_{k}$ are elements of a (column) vector $\mathbf{v}$, the function $\varphi$ can be written as the matrix product

$$
\varphi=\sum_{k=1}^{n} v_{k}^{2}=\left[\begin{array}{llll}
v_{1} & v_{2} & \cdots & v_{n}
\end{array}\right]\left[\begin{array}{c}
v_{1} \\
v_{2} \\
\vdots \\
v_{n}
\end{array}\right]=\mathbf{v}^{T} \mathbf{v}
$$

In the Line of Best Fit (unequal weights), we used the least squares function

$$
\varphi=\text { the sum of the weighted squared residuals }=\sum_{k=1}^{n} w_{k} v_{k}^{2}
$$

If the residuals $v_{k}$ are elements of a (column) vector $\mathbf{v}$ and the weights are the diagonal elements of a diagonal weight matrix $\mathbf{W}$, the function $\varphi$ can be written as the matrix product

$$
\varphi=\sum_{k=1}^{n} w_{k} v_{k}^{2}=\left[\begin{array}{llll}
v_{1} & v_{2} & \cdots & v_{n}
\end{array}\right]\left[\begin{array}{cccc}
w_{1} & 0 & 0 & 0 \\
0 & w_{2} & 0 & 0 \\
0 & 0 & \ddots & 0 \\
0 & 0 & 0 & w_{n}
\end{array}\right]\left[\begin{array}{c}
v_{1} \\
v_{2} \\
\vdots \\
v_{n}
\end{array}\right]=\mathbf{v}^{T} \mathbf{W} \mathbf{v}
$$

Note that in this example the weight matrix $\mathbf{W}$ represents a set of uncorrelated measurements.

In general, we may write least squares function as a matrix equation

$$
\begin{equation*}
\varphi=\mathbf{v}^{T} \mathbf{W} \mathbf{v} \tag{2.36}
\end{equation*}
$$

Note that replacing $\mathbf{W}$ with the identity matrix $\mathbf{I}$ gives the function for the case of equal weights and that for $n$ observations, the order of $\mathbf{v}$ is $(n, 1)$, the order of $\mathbf{W}$ is $(n, n)$ and the function $\varphi=\mathbf{v}^{T} \mathbf{W v}$ is a scalar quantity (a single number).

In both examples of the Line of Best Fit an observation equation $y_{k}+v_{k}=m x_{k}+c$ was used that if re-arranged as $v_{k}-m x_{k}+c=-y_{k}$ yields five equations for the coordinate pairs

$$
\begin{aligned}
& v_{1}-m x_{1}-c=-y_{1} \\
& v_{2}-m x_{2}-c=-y_{2} \\
& v_{3}-m x_{3}-c=-y_{3} \\
& v_{4}-m x_{4}-c=-y_{4} \\
& v_{5}-m x_{5}-c=-y_{5}
\end{aligned}
$$

Note that these re-arranged observation equations have all the unknown quantities $v, m$ and $c$ on the left of the equals sign and all the known quantities on the right.

These equations can be written in matrix form

$$
\left[\begin{array}{c}
v_{1} \\
v_{2} \\
\vdots \\
v_{5}
\end{array}\right]+\left[\begin{array}{cc}
-x_{1} & -1 \\
-x_{2} & -1 \\
\vdots & \vdots \\
-x_{5} & -1
\end{array}\right]\left[\begin{array}{l}
m \\
c
\end{array}\right]=\left[\begin{array}{c}
-y_{1} \\
-y_{2} \\
\vdots \\
-y_{5}
\end{array}\right]
$$

and written symbolically as

$$
\begin{gather*}
\mathbf{v}+\mathbf{B x}=\mathbf{f}  \tag{2.37}\\
\mathbf{f}=\mathbf{d}-\mathbf{l} \tag{2.38}
\end{gather*}
$$

If $n$ is the number of observations (equal to the number of equations) and $u$ is the number of unknown parameters
$\mathbf{v}$ is an $(n, 1)$ vector of residuals,
B is an $(n, u)$ matrix of coefficients,
$\mathbf{x} \quad$ is the $(u, 1)$ vector of unknown parameters,
f is the $(n, 1)$ vector of numeric terms derived from the observations,
d is an $(n, 1)$ vector of constants and
$\mathbf{l}$ is the ( $n, 1$ ) vector of observations.
Note that in many least squares problems the vector $\mathbf{d}$ is zero.

By substituting (2.37) into (2.36), we can obtain an expression for the least squares function

$$
\begin{aligned}
\varphi & =\mathbf{v}^{T} \mathbf{W} \mathbf{v} \\
& =(\mathbf{f}-\mathbf{B} \mathbf{x})^{T} \mathbf{W}(\mathbf{f}-\mathbf{B} \mathbf{x}) \\
& =\left(\mathbf{f}^{T}-(\mathbf{B} \mathbf{x})^{T}\right) \mathbf{W}(\mathbf{f}-\mathbf{B} \mathbf{x}) \\
& =\left(\mathbf{f}^{T}-\mathbf{x}^{T} \mathbf{B}^{T}\right) \mathbf{W}(\mathbf{f}-\mathbf{B x})
\end{aligned}
$$

and multiplication, observing the rule of matrix algebra gives

$$
\begin{equation*}
\varphi=\mathbf{f}^{T} \mathbf{W} \mathbf{f}-\mathbf{f}^{T} \mathbf{W B x}-\mathbf{x}^{T} \mathbf{B}^{T} \mathbf{W} \mathbf{f}+\mathbf{x}^{T} \mathbf{B}^{T} \mathbf{W B} \mathbf{x} \tag{2.39}
\end{equation*}
$$

Since $\varphi$ is a scalar (a number), the four terms on the right-hand-side of (2.39) are also scalars. Furthermore, since the transpose of a scalar is equal to itself, the second and third terms are equal $\left(\mathbf{f}^{T} \mathbf{W B x}\right)^{T}=\mathbf{x}^{T} \mathbf{B}^{T} \mathbf{W} \mathbf{f}$, remembering that $\mathbf{W}$ is symmetric hence $\mathbf{W}=\mathbf{W}^{T}$, giving

$$
\begin{equation*}
\varphi=\mathbf{f}^{T} \mathbf{W} \mathbf{f}-2 \mathbf{f}^{T} \mathbf{W B x}+\mathbf{x}^{T}\left(\mathbf{B}^{T} \mathbf{W} \mathbf{B}\right) \mathbf{x} \tag{2.40}
\end{equation*}
$$

In equation (2.40) all matrices and vectors are numerical constants except $\mathbf{x}$, the vector of unknown parameters, therefore for the least squares function $\varphi$ to be a minimum, its partial derivative with respect to each element in vector $\mathbf{x}$ must be equated to zero, i.e., $\varphi$ will be a minimum when $\frac{\partial \varphi}{\partial \mathbf{x}}=\mathbf{0}^{T}$. The first term of (2.40) does not contain $\mathbf{x}$ so its derivative is automatically zero and the second and third terms are bilinear and quadratic forms respectively and their derivatives are given in Appendix A, hence $\varphi$ will be a minimum when

$$
\frac{\partial \varphi}{\partial \mathbf{x}}=-2 \mathbf{f}^{T} \mathbf{W B}+2 \mathbf{x}^{T}\left(\mathbf{B}^{T} \mathbf{W B}\right)=\mathbf{0}^{T}
$$

Cancelling the 2's, re-arranging and transposing gives a set of normal equations

$$
\begin{equation*}
\left(\mathbf{B}^{T} \mathbf{W B}\right) \mathbf{x}=\mathbf{B}^{T} \mathbf{W} \mathbf{f} \tag{2.41}
\end{equation*}
$$

Equation (2.41) is often given in the form

$$
\begin{equation*}
\mathbf{N} \mathbf{x}=\mathbf{t} \tag{2.42}
\end{equation*}
$$

where

$$
\begin{array}{ll}
\mathbf{N}=\mathbf{B}^{T} \mathbf{W B} & \begin{array}{l}
\text { is a }(u, u) \text { coefficient matrix (the normal equation coefficient } \\
\\
\\
\\
\text { matrix), }
\end{array} \\
\mathbf{x} & \text { is the }(u, 1) \text { vector of unknown parameters and } \\
\mathbf{t}=\mathbf{B}^{T} \mathbf{W f} & \text { is a }(u, 1) \text { vector of numeric terms. }
\end{array}
$$

The solution for the vector of parameters $\mathbf{x}$ is given by

$$
\begin{equation*}
\mathbf{x}=\mathbf{N}^{-1} \mathbf{t} \tag{2.43}
\end{equation*}
$$

After solving for the vector $\mathbf{x}$, the residuals are obtained from

$$
\begin{equation*}
\mathbf{v}=\mathbf{f}-\mathbf{B x} \tag{2.44}
\end{equation*}
$$

and the vector of "adjusted" or estimated observations $\hat{\mathbf{l}}$ is

$$
\begin{equation*}
\hat{\mathbf{l}}=\mathbf{l}+\mathbf{v} \tag{2.45}
\end{equation*}
$$

The "hat" symbol ( $\wedge$ ) is used to denote quantities that result from a least squares process. Such quantities are often called adjusted quantities or least squares estimates.

These equations are the standard matrix solution for
least squares adjustment of indirect observations.

The name "least squares adjustment of indirect observations", adopted by Mikhail (1976) and Mikhail \& Gracie (1981), recognises the fact that each observation is an indirect measurement of the unknown parameters. This is the most common technique employed in surveying and geodesy and is described by various names, such as
parametric least squares
least squares adjustment by observation equations
least squares adjustment by residual equations

The technique of least squares adjustment of indirect observations has the following characteristics

- A mathematical model (equation) links observations, residuals (corrections) and unknown parameters.
- For $n$ observations, there is a minimum number $n_{0}$ required to determine the $u$ unknown parameters. In this case $n_{0}=u$ and the number of redundant observations is $r=n-n_{0}$.
- An equation can be written for each observation, i.e., there are $n$ observation equations. These equations can be represented in a standard matrix form; see equation (2.37), representing $n$ equations in $u$ unknowns and solutions for the unknown parameters, residuals and adjusted observations obtained from equations (2.41) to (2.45).

The popularity of this technique of adjustment is due to its easy adaptability to computerprogrammed solutions. As an example, the following MATLAB program best_fit_line.m reads a text file containing coordinate pairs (measurements) $x$ and $y$ and a weight $w$ (a measure of precision associated with each coordinate pair) and computes the parameters $m$ and $c$ of a line of best fit $y=m x+c$.

## MATLAB program best_fit_line

```
function best_fit_line
%
% BEST_FIT_LINE reads an ASCII textfile containing coordinate pairs (x,y)
% and weights (w) associated with each pair and computes the parameters
% m and c of the line of best fit y = mx + c using the least squares
% principle. Results are written to a textfile having the same path and
% name as the data file but with the extension ".out"
```

```
Function: best_fit_line
% Author:
    Rod Deakin,
    Department of Geospatial Science, RMIT University,
    GPO Box 2476V, MELBOURNE VIC 3001
    AUSTRALIA
    email: rod.deakin@rmit.edu.au
Date:
    Version 1.0 18 March 2003
```

\%
Remarks:
This function reads numeric data from a textfile containing coordinate
pairs ( $x, y$ ) and weights (w) associated with each pair and computes the
parameters $m$ and $c$ of a line of best fit $y=m x+c$ using the least
squares principle. Results are written to a textfile having the same
path and name as the data file but with the extension ".out"
Arrays:
$B \quad-(n, u)$ coeff matrix of observation equation $v+B x=f$
$\mathrm{f} \quad-\quad(\mathrm{n}, 1)$ vector of numeric terms
$N \quad-\quad(u, u)$ coefficient matrix of Normal equations $N x=t$
Ninv - ( $u, u$ ) inverse of $N$
$t \quad-\quad(u, 1)$ vector of numeric terms of Normal equations $N x=t$
$v \quad-\quad(n, 1)$ vector of residuals
W - (n,n) weight matrix
weight - $(n, 1)$ vector of weights
$x \quad-(u, 1)$ vector of solutions
x_coord - $(n, 1)$ vector of $x$ coordinates
y_coord - ( $n, 1$ ) vector of $y$ coordinates
Variables
n - number of equations
u - number of unknowns
References:
Notes on Least Squares (2003), Department of Geospatial Science, RMIT
University, 2003
\%

```
%------------------------------------------------------------------------
% 1. Call the User Interface (UI) to choose the input data file name
% 2. Concatenate strings to give the path and file name of the input file
% 3. Strip off the extension from the file name to give the rootName
% 4. Add extension ".out" to rootName to give the output filename
5. Concatenate strings to give the path and file name of the output file
filepath = strcat('c:\temp\','*.dat');
[infilename,inpathname] = uigetfile(filepath);
infilepath = strcat(inpathname,infilename);
rootName = strtok(infilename,'.');
```


## MATLAB program best_fit_line

```
outfilename = strcat(rootName,'.out');
outfilepath = strcat(inpathname,outfilename);
```

\%----------------------------------------------------------
\% 1. Load the data into an array whose name is the rootName
\% 2. set fileTemp = rootName
\% 3. Copy columns of data into individual arrays

load(infilepath);
fileTemp = eval(rootName);
x_coord = fileTemp(:,1);
y_coord = fileTemp(:,2);
weight = fileTemp(:,3);
\% determine the number of equations
n = length(x_coord);
\% set the number of unknowns
u = 2;
\% set the elements of the weight matrix $W$
$W=\operatorname{zeros}(n, n)$;
for $k=1: n$
w(k,k) = weight(k);
end
\% form the coefficient matrix $B$ of the observation equations
B = zeros(n,u);
for $k=1$ : $n$
$B(k, 1)=-x \_c o o r d(k)$;
$B(k, 2)=-1$;
end
\% for the vector of numeric terms $f$
$f=\operatorname{zeros}(n, 1)$;
for $k=1: n$
$f(k, 1)=-y \_c o o r d(k) ;$
end
\% form the normal equation coefficient matrix N
N = B'*W*B;
\% form the vector of numeric terms t
$t=B^{\prime *} W^{*} f$;
\% solve the system $N x=t$ for the unknown parameters $x$
Ninv = inv(N);
x = Ninv*t;
\% compute residuals
$v=f$ - ( $\mathrm{B}^{*} \mathrm{X}$ ) ;
\% open the output file print the data
fidout = fopen(outfilepath,'wt');
fprintf(fidout,'\n\nLine of Best Fit Least Squares Solution');
fprintf(fidout,'\n\nInput Data');
fprintf(fidout,'\n $x(k) \quad y(k) \quad$ weight $w(k) ')$;
for $k=1$ : $n$
fprintf(fidout,'\n\%10.4f \%10.4f \%10.4f',x_coord(k),y_coord(k), weight(k));
end

## MATLAB program best_fit_line

```
fprintf(fidout,'\n\nCoefficient matrix B of observation equations v + Bx = f');
for j = 1:n
    fprintf(fidout,'\n');
    for k = 1:u
        fprintf(fidout,'%10.4f',B(j,k));
    end
end
fprintf(fidout,'\n\nvector of numeric terms f of observation equations v + Bx =
f');
for k = 1:n
    fprintf(fidout,'\n%10.4f',f(k,1));
end
fprintf(fidout,'\n\nCoefficient matrix N of Normal equations Nx = t');
for j = 1:u
    fprintf(fidout,'\n');
    for k = 1:u
        fprintf(fidout,'%12.4f',N(j,k));
    end
end
fprintf(fidout,'\n\nvector of numeric terms t of Normal equations Nx = t');
for k = 1:u
    fprintf(fidout,'\n%10.4f',t(k,1));
end
fprintf(fidout,'\n\nInverse of Normal equation coefficient matrix');
for j = 1:u
    fprintf(fidout,'\n');
    for k = 1:u
        fprintf(fidout,'%16.4e',Ninv(j,k));
    end
end
fprintf(fidout,'\n\nVector of solutions x');
for k = 1:u
    fprintf(fidout,'\n%10.4f',x(k,1));
end
fprintf(fidout,'\n\nVector of residuals v');
for k = 1:n
    fprintf(fidout,'\n%10.4f',v(k,1));
end
fprintf(fidout,'\n\n');
% close the output file
fclose(fidout);
```

MATLAB program best_fit_line
Data file c:\Temp\line_data.dat

```
% data file for function "best_fit_line.m"
% x y w
    -40.0 -24.0 2
    -15.0 -24.0 5
    10.0 -12.0 7
    38.0 15.0 3
    67.0 30.0 3
```


## MATLAB program best_fit_line

Running the program from the MATLAB command window prompt >> opens up a standard Microsoft Windows file selection window in the directory c:\Temp. Select the appropriate data file (in this example: line_data.dat) by double clicking with the mouse and the program reads the data file, computes the solutions and writes the output data to the file c: \Temp\line_data.out

## MATLAB command window



## MATLAB program best_fit_line

Output file c:\Temp\line_data.out

```
Line of Best Fit Least Squares Solution
Input Data
        x(k) y(k) weight w(k)
    -40.0000 -24.0000 2.0000
    -15.0000 -24.0000 5.0000
    10.0000 -12.0000 7.0000
    38.0000 15.0000 3.0000
    67.0000 30.0000 3.0000
Coefficient matrix B of observation equations v + Bx = f
    40.0000 -1.0000
    15.0000 -1.0000
    -10.0000 -1.0000
    -38.0000 -1.0000
    -67.0000 -1.0000
Vector of numeric terms f of observation equations v + Bx = f
    24.0000
    24.0000
    12.0000
    -15.0000
    -30.0000
Coefficient matrix N of Normal equations Nx = t
    22824.0000 230.0000
        230.0000 20.0000
Vector of numeric terms t of Normal equations Nx = t
10620.0000
    -117.0000
Inverse of Normal equation coefficient matrix
            4.9556e-005 -5.6990e-004
            -5.6990e-004 5.6554e-002
Vector of solutions x
        0.5930
    -12.6691
Vector of residuals v
    -12.3878
        2.4363
        5.2605
        -5.1363
        -2.9403
```

The data in this example is taken from section 2.4.2 Line of Best Fit (unequal weights)

## MATLAB program best_fit_line

By adding the following lines to the program, the Line of Best Fit is shown on a plot together with the data points.

```
%--------------------------------------
% plot data points and line of best fit
%-----------------------------------------
% copy solutions from vector x
m = x(1,1);
c = x(2,1);
% find minimum and maximum x coordinates
xmin = min(x_coord);
xmax = max(x_coord);
% create a vector of x coordinates at intervals of 0.1
% between min and max coordinates
x = xmin:0.1:xmax;
% calculate y coordinates of Line of Best Fit
y = m*x + c;
% Select Figure window and clear figure
figure(1);
clf(1);
hold on;
grid on;
box on;
% plot line of best fit and then the data points with a star (*)
plot(x,y,'k-');
plot(x_coord,y_coord,'k*');
% anotate the plot
title('Least Squares Line of Best Fit')
xlabel('X coordinate');
ylabel('Y coordinate');
```



Figure 2.3 Least Squares Line of Best Fit

### 2.7. Least Squares Curve Fitting

The general matrix solutions for least squares adjustment of indirect observations (see equations (2.37) to (2.45) of section 2.6) can be applied to curve fitting. The following two examples (parabola and ellipse) demonstrate the technique.

### 2.7.1. Least Squares Best Fit Parabola

Consider the following: A surveyor working on the re-alignment of a rural road is required to fit a parabolic vertical curve such that it is a best fit to the series of natural surface Reduced Levels (RL's) on the proposed new alignment. Figure 2.2 shows a Vertical Section of the proposed alignment with Chainages ( $x$-values) and RL's ( $y$-values).


Figure 2.2 Vertical Section of proposed road alignment

The general equation of a parabolic curve is

$$
\begin{equation*}
y=a x^{2}+b x+c \tag{2.46}
\end{equation*}
$$

This is the mathematical model that we assume our data accords with and to account for the measurement inconsistencies, due to the irregular natural surface and small measurement errors we can add residuals to the left-hand-side of (2.46) to give an observation equation

$$
\begin{equation*}
y_{k}+v_{k}=a x_{k}^{2}+b x_{k}+c \tag{2.47}
\end{equation*}
$$

Equation (2.47) can be re-arranged as

$$
\begin{equation*}
v_{k}-a x_{k}^{2}-b x-c=-y_{k} \tag{2.48}
\end{equation*}
$$

$n=6$ equations in $u=3$ unknown parameters $a, b, c$ can be written in matrix form $\mathbf{v}+\mathbf{B x}=\mathbf{f}$ as

$$
\left[\begin{array}{c}
v_{1} \\
v_{2} \\
\vdots \\
v_{6}
\end{array}\right]+\left[\begin{array}{ccc}
-x_{1}^{2} & -x_{1} & -1 \\
-x_{2}^{2} & -x_{2} & -1 \\
\vdots & \vdots & \vdots \\
-x_{6}^{2} & -x_{6} & -1
\end{array}\right]\left[\begin{array}{l}
a \\
b \\
c
\end{array}\right]=\left[\begin{array}{c}
-y_{1} \\
-y_{2} \\
\vdots \\
-y_{6}
\end{array}\right]
$$

where

$$
\mathbf{v}_{(6,1)}=\left[\begin{array}{c}
v_{1} \\
v_{2} \\
\vdots \\
v_{6}
\end{array}\right], \quad \mathbf{B}_{(6,3)}=\left[\begin{array}{ccc}
-x_{1}^{2} & -x_{1} & -1 \\
-x_{2}^{2} & -x_{2} & -1 \\
\vdots & \vdots & \vdots \\
-x_{6}^{2} & -x_{6} & -1
\end{array}\right], \quad \mathbf{x}_{(3,1)}=\left[\begin{array}{l}
a \\
b \\
c
\end{array}\right], \quad \mathbf{f}_{(6,1)}=\left[\begin{array}{c}
-y_{1} \\
-y_{2} \\
\vdots \\
-y_{6}
\end{array}\right]
$$

Considering all the measurements to be of equal precision, i.e., $\mathbf{W}=\mathbf{I}$, the least squares solution for the three parameters in the vector $\mathbf{x}$ is given by the following sequence of operations

- form the normal coefficient matrix: $\mathbf{N}=\mathbf{B}^{T} \mathbf{W B}$
- form the vector of numeric terms: $\mathbf{t}=\mathbf{B}^{T} \mathbf{W f}$
- compute the matrix inverse: $\mathbf{N}^{-1}$
- compute the solutions: $\quad \mathbf{x}=\mathbf{N}^{-1} \mathbf{t}$
- compute the residuals:

$$
\mathbf{v}=\mathbf{f}-\mathbf{B} \mathbf{x}
$$

This is the identical series of operations to solve for the parameters of the Line of Best Fit, except in this case $u=3$. With minor modifications to the MATLAB program best_fit_line.m another MATLAB program best_fit_parabola.m can be created to determine the parameters $a$, $b, c$ of the best fit parabola. The relevant modifications are shown below.

## MATLAB program best_fit_parabola

Making the following changes to the MATLAB program best_fit_line, a new program best_fit_parabola can be created.

Changes to function name and help instructions

```
function best_fit_parabola
%
% BEST_FIT_PARABOLA reads an ASCII textfile containing coordinate pairs (x,y)
% and weights (w) associated with each pair and computes the parameters
% a, b and c of a best fit parabola y = a( }\mp@subsup{x}{*}{*}x)+bx+cusing the leas
% squares principle. Results are written to a textfile having the same
% path and name as the data file but with the extension ".out"
```

Changes to function remarks in documentation section

```
% Remarks:
% This function reads numeric data from a textfile containing coordinate
% pairs (x,y) and weights (w) associated with each pair and computes the
% parameters a, b, and c of a best fit parabola y = a(x*x) + bx + c using
% the least squares principle. Results are written to a textfile having
% the same path and name as the data file but with the extension ".out"
```

Changes to formation of coefficient matrix B

```
% form the coefficient matrix B of the observation equations
B = zeros(n,u);
for k = 1:n
    B(k,1) = - (x_coord(k)^2);
    B(k,2) = -x_coord(k);
    B}(\textrm{k},3)=-1
end
```

Changes to data plotting section

```
%------------------------------------------
% plot data points and Parabola of best fit
%---------------------------------------------
% copy solutions from vector x
a = x(1,1);
b = x(2,1);
c = x(3,1);
% find minimum and maximum x coordinates
xmin = min(x_coord);
xmax = max(x_coord);
% create a vector of x coordinates at intervals of 0.1
% between min and max coordinates
x = xmin:0.1:xmax;
% calculate y coordinates of Parabola of Best Fit
y = a*(x.*x) + b*x + c;
```


## MATLAB program best_fit_parabola

Using the data from Figure 2.2 a data file c:\Temp\parabola_data.dat was created

| data |  |  |  |
| :---: | :---: | :---: | :---: |
| $\%$ | file for | function "best_fit_parabola.m" |  |
| \% | y | w |  |
| 100.0 | 63.48 | 1 |  |
| 150.0 | 46.20 | 1 |  |
| 200.0 | 36.62 | 1 |  |
| 250.0 | 38.96 | 1 |  |
| 300.0 | 47.42 | 1 |  |
| 350.0 | 57.72 | 1 |  |

Running the program from the MATLAB command window generated the following output file c:\Temp \parabola_data. out and a plot of the Least Squares Parabola of best Fit

```
Parabola of Best Fit Least Squares Solution
Input Data
        x(k) y(k) weight w(k)
    100.0000
    150.0000
    200.0000
    250.0000
    300.0000
    350.0000
        63.4800 1.0000
        36.6200 1.0000
        38.9600 1.0000
        47.4200 1.0000
        57.7200 1.0000
Coefficient matrix B of observation equations v + Bx = f
        -10000.0000
                -100.0000
        -1.0000
        -22500.0000 -150.0000 -1.0000
        -40000.0000 -200.0000 -1.0000
        -62500.0000 -250.0000 -1.0000
        -90000.0000 -300.0000 -1.0000
        -122500.0000 -350.0000 -1.0000
Vector of numeric terms f of observation equations v + Bx = f
            -63.4800
            -46.2000
            -36.6200
            -38.9600
            -47.4200
            -57.7200
Coefficient matrix N of Normal equations Nx = t
29218750000.0000 97875000.0000 347500.0000
        97875000.0000 347500.0000 1350.0000
            347500.0000 1350.00000 6.0000
Vector of numeric terms t of Normal equations Nx = t
    16912600.0000
        64770.0000
            290.4000
Inverse of Normal equation coefficient matrix
        4.2857e-009 -1.9286e-006 1.8571e-004
        -1.9286e-006 8.9071e-004 -8.8714e-002
        1.8571e-004 -8.8714e-002 9.3714e+000
Vector of solutions x
            0.001500
            -0.688221
        116.350000
```


## MATLAB program best_fit_parabola

```
Vector of residuals v
    -0.948
        0.676
        2.103
    -0.889
    -2.498
    1.555
```



Figure 2.4 Least Squares Parabola of Best Fit

### 2.7.2. Least Squares Best Fit Ellipse

In November 1994, a survey was undertaken by staff of the Department of Geospatial Science at the Melbourne Cricket Ground (MCG) to determine the dimensions of the playing surface. This survey was to decide which of two sets of dimensions was correct, those of the Melbourne Cricket Club (MCC) or those of the Australian Football League (AFL). The MCC curator Tony Ware and the AFL statistician Col Hutchison both measured the length of the ground (Tony Ware with a 100-metre nylon tape and Col Hutchison with a measuring wheel) and compared their distances with the "true" distance determined by Electronic Distance Measurement (EDM) with a Topcon 3B Total Station. Their measurements were both reasonably close to the EDM distance and it turned out that the "official" AFL dimensions
were incorrect. After this "measure-off", observations (bearings and distances) were made to seventeen points around the edge of the playing surface to determine the Least Squares Ellipse of Best Fit and to see if the major axis of this ellipse was the actual line between the goals at either end. The Total Station was set-up close to the goal-to-goal axis and 20-25 metres from the centre of the ground. An arbitrary $X, Y$ coordinate system was used with the origin at the Total Station and the positive $X$-axis in the direction of the Brunton Avenue end of the Great Southern Stand (approximately west). The table of coordinates is given below; point numbers 1 to 6 were not points on the edge of the ground.

| Point No. | $X$-coordinate | $Y$-coordinate |
| :---: | :---: | :---: |
| 7 | -54.58 | 17.11 |
| 8 | -45.47 | 36.56 |
| 9 | -28.40 | 53.22 |
| 10 | -2.02 | 63.72 |
| 11 | 28.12 | 63.44 |
| 12 | 57.49 | 52.55 |
| 13 | 80.85 | 34.20 |
| 14 | 98.08 | 9.14 |
| 15 | 105.69 | -17.30 |
| 16 | 103.83 | -46.96 |
| 17 | 88.42 | -71.50 |
| 18 | 61.26 | -86.84 |
| 19 | 26.47 | -91.07 |
| 20 | -6.59 | -81.37 |
| 21 | -34.55 | -59.24 |
| 22 | -51.51 | -29.28 |
| 23 | -56.30 | -2.31 |

Table 2.4 Arbitrary coordinates of points around the perimeter of the playing surface of the MCG (date of survey November 1994)

To develop an observation equation for the Least Squares Ellipse of Best Fit and to determine the lengths and directions of the axes of the ellipse the following derivation of the general equation of an ellipse is necessary.

Figure 2.5 shows an ellipse whose axes are aligned with the $u-v$ axes. The semi-axes lengths are $a$ and $b(a>b)$, the centre of the ellipse is at $X_{0}, Y_{0}$ and the ellipse axes are rotated by an
angle $\beta$, measured positive anti-clockwise from the $x$-axis. The $x$ - $y$ axes are parallel to the $X$ $Y$ axes and pass through the centre of the ellipse.


Figure 2.5

The $u, v$ Cartesian equation of the ellipse is

$$
\begin{equation*}
\frac{u^{2}}{a^{2}}+\frac{v^{2}}{b^{2}}=1 \tag{2.49}
\end{equation*}
$$

Equation (2.49) can be expressed in matrix form as

$$
\left[\begin{array}{ll}
u & v
\end{array}\right]\left[\begin{array}{cc}
1 / a^{2} & 0  \tag{2.50}\\
0 & 1 / b^{2}
\end{array}\right]\left[\begin{array}{l}
u \\
v
\end{array}\right]=1
$$

The $u, v$ axes are rotated (positive anti-clockwise) by an angle $\beta$ from the $x, y$ axes and the relationship between coordinates is shown in Figure 2.6


Figure 2.6

Inspection of Figure 2.6 shows

$$
\begin{align*}
& u=x \cos \beta+y \sin \beta \\
& v=-x \sin \beta+y \cos \beta \tag{2.51}
\end{align*}
$$

Replacing $\cos \beta$ and $\sin \beta$ with the letters c and s the coordinate relationships can be represented as a matrix equation

$$
\left[\begin{array}{l}
u  \tag{2.52}\\
v
\end{array}\right]=\left[\begin{array}{rr}
\mathrm{c} & \mathrm{~s} \\
-\mathrm{s} & \mathrm{c}
\end{array}\right]\left[\begin{array}{l}
x \\
y
\end{array}\right]
$$

Transposing this equation (remembering the reversal rule with the transpose of matrix products) gives

$$
\left[\begin{array}{ll}
u & v
\end{array}\right]=\left[\begin{array}{ll}
x & y
\end{array}\right]\left[\begin{array}{rr}
\mathrm{c} & -\mathrm{s}  \tag{2.53}\\
\mathrm{~s} & \mathrm{c}
\end{array}\right]
$$

Substituting (2.52) and (2.53) into (2.50) and multiplying the matrices gives

$$
\begin{array}{r}
{\left[\begin{array}{ll}
x & y
\end{array}\right]\left[\begin{array}{rr}
\mathrm{c} & -\mathrm{s} \\
\mathrm{~s} & \mathrm{c}
\end{array}\right]\left[\begin{array}{cc}
1 / a^{2} & 0 \\
0 & 1 / b^{2}
\end{array}\right]\left[\begin{array}{rr}
\mathrm{c} & \mathrm{~s} \\
-\mathrm{s} & \mathrm{c}
\end{array}\right]\left[\begin{array}{l}
x \\
y
\end{array}\right]=1} \\
{\left[\begin{array}{ll}
x & y
\end{array}\right]\left[\begin{array}{l}
\left(\frac{\mathrm{c}^{2}}{a^{2}}+\frac{\mathrm{s}^{2}}{b^{2}}\right)\left(\frac{\mathrm{cs}}{a^{2}}-\frac{\mathrm{cs}}{b^{2}}\right) \\
\left(\frac{\mathrm{cs}}{a^{2}}-\frac{\mathrm{cs}}{b^{2}}\right)\left(\frac{\mathrm{s}^{2}}{a^{2}}+\frac{\mathrm{c}^{2}}{b^{2}}\right)
\end{array}\right]\left[\begin{array}{l}
x \\
y
\end{array}\right]=1}
\end{array}
$$

Replacing the elements of the square matrix with the symbols $A, B$ and $H$, noting that the topright and lower-left elements are the same, this equation may be written in a general form as

$$
\begin{gather*}
{\left[\begin{array}{ll}
x & y
\end{array}\right]\left[\begin{array}{ll}
A & H \\
H & B
\end{array}\right]\left[\begin{array}{l}
x \\
y
\end{array}\right]=1} \\
A x^{2}+2 H x y+B y^{2}=1 \tag{2.54}
\end{gather*}
$$

Equation (2.54) is the equation of an ellipse centred at the coordinate origin but with axes rotated from the $x, y$ axes. The semi axes lengths $a$ and $b$, and the rotation angle $\beta$ can be determined from (2.54) by the following method.

Letting $x=r \cos \theta$ and $y=r \sin \theta$ in equation (2.54) gives the polar equation of the ellipse

$$
\begin{equation*}
A \cos ^{2} \theta+2 H \cos \theta \sin \theta+B \sin ^{2} \theta=\frac{1}{r^{2}} \tag{2.55}
\end{equation*}
$$

$r$ is the radial distance from the centre of the ellipse and $\theta$ is the angle measured positive anti-clockwise from the $x$-axis. Equation (2.55) has maximum and minimum values defining the lengths and directions of the axes of the ellipse. To determine these values from (2.55), consider the following

Let

$$
\begin{aligned}
\frac{1}{r^{2}}=f & =A \cos ^{2} \theta+2 H \cos \theta \sin \theta+B \sin ^{2} \theta \\
& =A \cos ^{2} \theta+H \sin 2 \theta+B \sin ^{2} \theta
\end{aligned}
$$

and aim to find the optimal (maximum and minimum) values of $f$ and the values of $\theta$ when these occur by investigating the first and second derivatives $f^{\prime}$ and $f^{\prime \prime}$ respectively, i.e.,

$$
f \text { is }\left\{\begin{array}{c}
\max \\
\min
\end{array}\right\} \text { when }\left\{\begin{array}{c}
f^{\prime}=0 \text { and } f^{\prime \prime}<0 \\
f^{\prime}=0 \text { and } f^{\prime \prime}>0
\end{array}\right\}
$$

where

$$
\begin{equation*}
f^{\prime}=(B-A) \sin 2 \theta+2 H \cos 2 \theta \tag{2.56}
\end{equation*}
$$

Now the maximum or minimum value of $f$ occurs when $f^{\prime}=0$ and from the first member of (2.56) the value of $\theta$ is given by

$$
\begin{equation*}
\tan 2 \theta=\frac{2 H}{A-B} \tag{2.57}
\end{equation*}
$$

But this value of $\theta$ could relate to either a maximum or a minimum value of $f$. So from the second member of equations (2.56) with a value of $2 \theta$ from equation (2.57) this ambiguity can be resolved by determining the sign of the second derivative $f^{\prime \prime}$ giving $\left\{\begin{array}{c}f_{\text {max }} \\ f_{\text {min }}\end{array}\right\}$ when $\left\{\begin{array}{l}f^{\prime \prime}<0 \\ f^{\prime \prime}>0\end{array}\right\}$

In the polar equation of the ellipse given by equation (2.55) $f_{\max }$ coincides with $r_{\min }$ and $f_{\min }$ coincides with $r_{\max }$ so the angle $\beta$ (measured positive anti-clockwise) from the $x$-axis to the major axis of the ellipse (see Figure 2.5) is found from

$$
\left\{\begin{array}{l}
r_{\text {max }}  \tag{2.58}\\
r_{\text {min }}
\end{array}\right\} \text { when }\left\{\begin{array}{l}
f^{\prime \prime}>0 \\
f^{\prime \prime}<0
\end{array}\right\} \text { and }\left\{\begin{array}{l}
\beta=\theta \\
\beta=\theta-\frac{1}{2} \pi
\end{array}\right\}
$$

These results can be verified by considering the definitions of $A, B$ and $H$ used in the derivation of the polar equation of the ellipse, i.e.,

$$
A=\frac{\cos ^{2} \beta}{a^{2}}+\frac{\sin ^{2} \beta}{b^{2}}, B=\frac{\sin ^{2} \beta}{a^{2}}+\frac{\cos ^{2} \beta}{b^{2}}, \quad H=\frac{\cos \beta \sin \beta}{a^{2}}-\frac{\cos \beta \sin \beta}{b^{2}}
$$

and

$$
A-B=\left(\frac{1}{a^{2}}-\frac{1}{b^{2}}\right) \cos 2 \beta, 2 H=\left(\frac{1}{a^{2}}-\frac{1}{b^{2}}\right) \sin 2 \beta
$$

giving

$$
\tan 2 \beta=\frac{2 H}{A-B}
$$

Noting that the values of $\theta$ coinciding with the maximum or minimum values of the function $f$ are found from equation (2.57) then $\tan 2 \beta=\frac{2 H}{A-B}=\tan 2 \theta$ or

$$
\tan 2 \theta=\tan 2 \beta
$$

whereupon

$$
2 \theta=2 \beta+n \pi \text { or } \theta=\beta+\frac{1}{2} n \pi \text { where } n \text { is an integer }
$$

Also, from the second member of equations (2.56)

$$
f^{\prime \prime}=2(B-A) \cos 2 \theta-4 H \sin 2 \theta
$$

Now, for $n=0$

$$
\theta=\beta,\left.f^{\prime \prime}\right|_{\theta=\beta}=-2\left(\frac{1}{a^{2}}-\frac{1}{b^{2}}\right) \text { and since } a>b,\left.f^{\prime \prime}\right|_{\theta=\beta}>0
$$

So $\theta=\beta$ makes $f$ minimum and so $r$ is maximum and

$$
\begin{aligned}
f_{\min } & =A \cos ^{2} \beta+2 H \sin \beta \cos \beta+B \sin ^{2} \beta \\
& =\frac{\left(\cos ^{2} \beta+\sin ^{2} \beta\right)^{2}}{a^{2}}=\frac{1}{a^{2}}
\end{aligned}
$$

$$
\text { So } r_{\text {max }}=a
$$

When $n=1$
$\theta=\beta+\frac{1}{2} \pi, \sin 2 \theta=-\sin 2 \beta, \cos 2 \theta=-\cos 2 \beta$ and so

$$
\left.f^{\prime \prime}\right|_{\theta=\beta+\frac{1}{2} \pi}=2\left(\frac{1}{a^{2}}-\frac{1}{b^{2}}\right) \text { and since } a>b,\left.f^{\prime \prime}\right|_{\theta=\beta+\frac{1}{2} \pi}<0
$$

So $\theta=\beta+\frac{1}{2} \pi$ makes $f$ maximum and so $r$ is minimum and

$$
\begin{aligned}
& f_{\max }=\frac{\left(\sin ^{2} \beta+\cos ^{2} \beta\right)^{2}}{b^{2}}=\frac{1}{b^{2}} \\
& \text { So } r_{\min }=b
\end{aligned}
$$

When $n=2$

$$
\begin{aligned}
& \theta=\beta+\pi, \sin 2 \theta=\cos 2 \beta, \cos 2 \theta=\cos 2 \beta \text { and }\left.f^{\prime \prime}\right|_{\theta=\beta+\pi}>0 \\
& \text { So } \theta=\beta+\frac{1}{2} \pi \text { makes } f_{\min }=\frac{1}{a^{2}} \text { and } r_{\max }=a
\end{aligned}
$$

When $n=3$

$$
\begin{aligned}
& \theta=\beta+\frac{3}{2} \pi, \sin 2 \theta=-\cos 2 \beta, \cos 2 \theta=-\cos 2 \beta \text { and }\left.f^{\prime \prime}\right|_{\theta=\beta+\frac{3}{2} \pi}<0 \\
& \text { So } \theta=\beta+\frac{3}{2} \pi \text { makes } f_{\max }=\frac{1}{b^{2}} \text { and } r_{\min }=b
\end{aligned}
$$

All other even values of $n$ give the same result as $n=2$ and all other odd values of $n$ give the same result as $n=1$

Now consider Figure 2.5 and the general Cartesian equation of the ellipse, re-stated again as

$$
\begin{equation*}
a X^{2}+2 h X Y+b Y^{2}+d X+e Y=1 \tag{2.59}
\end{equation*}
$$

where the translated $x, y$ coordinate system is related to the $X, Y$ system by

$$
X=x+X_{0} \quad \text { and } \quad Y=y+Y_{0}
$$

Substituting these relationships into (2.59) gives

$$
a\left(x+X_{0}\right)^{2}+2 h\left(x+X_{0}\right)\left(y+Y_{0}\right)+b\left(y+Y_{0}\right)^{2}+d\left(x+X_{0}\right)+e\left(y+Y_{0}\right)=1
$$

Expanding and gathering terms gives

$$
\begin{aligned}
a x^{2}+2 h x y+b y^{2} & +\left(2 a X_{0}+2 h Y_{0}+d\right) x \\
& +\left(2 a Y_{0}+2 h X_{0}+e\right) y \\
& +a X_{0}^{2}+2 h X_{0} Y_{0}+b Y_{0}^{2}+d X_{0}+e Y_{0}=1
\end{aligned}
$$

Inspection of the left-hand-side of this equation reveals three parts:
(i) $a x^{2}+2 h x y+b y^{2}$ is the left-hand-side of the equation of an ellipse, similar in form to equation (2.54),
(ii) coefficient terms of $x$ and $y$; $\left(2 a X_{0}+2 h Y_{0}+d\right)$ and $\left(2 a Y_{0}+2 h X_{0}+e\right)$,
(iii) a constant term $a X_{0}^{2}+2 h X_{0} Y_{0}+b Y_{0}^{2}+d X_{0}+e Y_{0}$

Now when the coefficients of $x$ and $y$ are zero the ellipse will be centred at the origin of the $x, y$ axes with an equation of the form

$$
\begin{equation*}
a x^{2}+2 h x y+b y^{2}=c \tag{2.60}
\end{equation*}
$$

where

$$
\begin{equation*}
c=1-\left(a X_{0}^{2}+2 h X_{0} Y_{0}+b Y_{0}^{2}+d X_{0}+e Y_{0}\right) \tag{2.61}
\end{equation*}
$$

and

$$
\begin{align*}
2 a X_{0}+2 h Y_{0}+d & =0  \tag{2.62}\\
2 h X_{0}+2 b Y_{0}+e & =0
\end{align*}
$$

Equations (2.62) can be written in matrix form and solved (using the inverse of a 2,2 matrix) to give $X_{0}$ and $Y_{0}$

$$
\begin{aligned}
& {\left[\begin{array}{l}
d \\
e
\end{array}\right]=\left[\begin{array}{ll}
-2 a & -2 h \\
-2 h & -2 b
\end{array}\right]\left[\begin{array}{l}
X_{0} \\
Y_{0}
\end{array}\right]} \\
& {\left[\begin{array}{c}
X_{0} \\
Y_{0}
\end{array}\right]=\frac{1}{2 a b-2 h^{2}}\left[\begin{array}{cc}
-b & h \\
h & -a
\end{array}\right]\left[\begin{array}{l}
d \\
e
\end{array}\right]}
\end{aligned}
$$

giving

$$
\begin{equation*}
X_{0}=\frac{e h-b d}{2\left(a b-h^{2}\right)} \quad \text { and } \quad Y_{0}=\frac{d h-a e}{2\left(a b-h^{2}\right)} \tag{2.63}
\end{equation*}
$$

Dividing both sides of (2.60) by $c$ gives

$$
\begin{equation*}
A x^{2}+2 H x y+B y^{2}=1 \tag{2.64}
\end{equation*}
$$

where

$$
A=\frac{a}{c}, \quad H=\frac{h}{c}, \quad B=\frac{b}{c}
$$

Equation (2.64), identical to equation (2.54), is the equation of an ellipse centred at the $x, y$ coordinate origin whose axes are rotated from the $x, y$ axes by an angle $\beta$. The rotation angle $\beta$ and semi-axes lengths $a$ and $b$ of the ellipse can be determined using the method set out above and equations (2.58), (2.57), (2.56) and (2.55). Thus, we can see from the development that the general Cartesian equation of an ellipse is given by

$$
\begin{equation*}
a X^{2}+2 h X Y+b Y^{2}+d X+e Y=1 \tag{2.65}
\end{equation*}
$$

Note that the coefficients $a$ and $b$ in this equation are not the semi-axes lengths of the ellipse.

Returning to the problem of the Least Squares Ellipse of Best Fit for the MCG, the size, shape location and orientation of this ellipse can be determined from a set of observation equations of the form

$$
\begin{equation*}
v_{k}+a X_{k}^{2}+2 h X_{k} Y_{k}+b Y_{k}^{2}+d X_{k}+e Y_{k}=1 \tag{2.66}
\end{equation*}
$$

This observation equation is the general Cartesian equation of an ellipse with the addition of the residual $v_{k}$. The addition of $v_{k}$ to the left-hand-side of (2.65) is simply a convenience and reflects the fact that the measured coordinates $X_{k}, Y_{k}$ are inconsistent with the mathematical model. For each of the 17 measured points around the perimeter of the MCG an equation can be written and arranged in the matrix form $\mathbf{v}+\mathbf{B x}=\mathbf{f}$

$$
\left[\begin{array}{c}
v_{1} \\
v_{2} \\
\vdots \\
v_{17}
\end{array}\right]+\left[\begin{array}{ccccc}
X_{1}^{2} & X_{1} Y_{1} & Y_{1}^{2} & X_{1} & Y_{1} \\
X_{2}^{2} & X_{2} Y_{2} & Y_{2}^{2} & X_{2} & Y_{2} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
X_{17}^{2} & X_{17} Y_{17} & Y_{17}^{2} & X_{17} & Y_{17}
\end{array}\right]\left[\begin{array}{c}
a \\
2 h \\
b \\
d \\
e
\end{array}\right]=\left[\begin{array}{c}
1 \\
1 \\
\vdots \\
1
\end{array}\right]
$$

The vector $\mathbf{x}$ contains the parameters $a, h, b, d$ and $e$ of the general equation of the ellipse and with a weight matrix $\mathbf{W}=\mathbf{I}$ (i.e., all observations of equal precision) the solution for $\mathbf{x}$ is given by the following sequence of operations

- form the normal coefficient matrix: $\mathbf{N}=\mathbf{B}^{T} \mathbf{W B}$
- form the vector of numeric terms: $\mathbf{t}=\mathbf{B}^{T} \mathbf{W f}$
- compute the matrix inverse: $\mathbf{N}^{-1}$
- compute the solutions: $\quad \mathbf{x}=\mathbf{N}^{-1} \mathbf{t}$
- compute the residuals:
$\mathbf{v}=\mathbf{f}-\mathbf{B x}$
This is the identical series of operations to solve for the parameters of the Line of Best Fit, and for the Parabola of Best Fit except in this case the residuals $\mathbf{v}$ have little practical meaning because they are not connected to quantities such as distances or coordinates. In the case of the Least Squares Ellipse of Best Fit, it is better to compute the offsets $h$ (perpendicular distances) from the ellipse to the data points rather than the residuals $\mathbf{v}$.

To compute offsets $h$ the following preliminary sequence of operations is required:
(i) compute the parameters $a, h, b, d$ and $e$ using the Least Squares process set out above.
(ii) compute the coordinates of the origin $X_{0}, Y_{0}$ and the constant $c$ using equations (2.63) and (2.61).
(iii) compute coefficients $A, H$ and $B$ of the ellipse given by (2.64) which can then be used to compute the rotation angle $\beta$ and the semi-axes lengths $a$ and $b$ from equations (2.55) to (2.58) and.
(iv) compute the $u, v$ coordinates of the data points using equations (2.51).

Now, having the $u, v$ coordinates, the offsets $h$ can be computed. Consider the sectional view of a quadrant of an ellipse in Figure 2.7. The $u, v$ axes are in the direction of the major and minor axes respectively ( $a$ and $b$ are the semi-axes lengths) and $P$ is a point related to the ellipse by the normal, which makes an angle $\phi$ with the major axis, and the distance $h=Q P$ along the normal. The $u, v$ coordinates of $P$ are the distances $L P$ and $M P$ respectively. From the geometry of an ellipse, the normal intersects the minor axis at $H$ and the distance $Q H=v$ (where $v$ is the Greek symbol $n u$ ) and the distances $D H$ and $O H$ are $v e^{2}$ and $v e^{2} \sin \phi$ respectively. $e$ is the eccentricity of the ellipse and the eccentricity and flattening $f$ of an ellipse are related to the semi-axes $a$ and $b$.


Figure $2.7 u, v$ coordinates of $P$ related to an ellipse $(a, b)$

The equations for $f, e^{2}$ and $v$ are

$$
\begin{aligned}
f & =\frac{a-b}{a} \\
e^{2} & =f(2-f) \\
v & =\frac{a}{\sqrt{1-e^{2} \sin ^{2} \phi}}
\end{aligned}
$$

Using these relationships, the angle $\phi$ and perpendicular distance $h$ are given by

$$
\begin{align*}
\tan \phi & =\frac{v+v e^{2} \sin \phi}{u}  \tag{2.67}\\
h & =\frac{u}{\cos \phi}-v \tag{2.68}
\end{align*}
$$

Inspecting these equations; if the semi-axes $a, b$ and the $u, v$ coordinates of $P$ are known, the perpendicular offset $h$ can be determined from (2.68) and (2.67). It should be noted that functions of $\phi$ appear on both sides of the equals sign of equation (2.67) and $\phi$ must be solved by iteration.

To determine the Least Square Best Fit Ellipse for the playing surface of the MCG a
MATLAB program best_fit_ellipse.m operating in the same way as the MATLAB programs best_fit_line and best_fit_parabola with a data file (in this example: MCG_ellipse_data.dat)

Data file c:\Temp\MCG_ellipse_data.dat

```
% Data file for MCG Survey, November 1994
% Coordinates of 17 boundary points (edge of concrete)
%
% point X Y weight
            -54.58 17.11 1
            -45.47 36.56 1
            -28.40 53.22 1
            -2.02 63.72 1
            28.12 63.44 1
                57.49 52.55 1
                80.85 34.20 1
            98.08 9.14
            105.69 -17.30
            103.83 -46.96 1
                88.42 -71.50 1
                61.26 -86.84 1
                26.47 -91.07 1
                -6.59 -81.37 1
            -34.55 -59.24 1
            -51.51 -29.28 1
            -56.30 -2.31 1
```

gives the following results (contained in an output file having the same name and path as the data file but with the extension .dat) and plot on the screen.

Output file c:\Temp\MCG_ellipse_data.out

| Ellipse of Best Fit Least Squares Solution |  |  |  |
| :---: | :---: | :---: | :---: |
| Input Data |  |  |  |
| point | $x(k)$ | $y(k)$ | weight w(k) |
| 7 | -54.5800 | 17.1100 | 1.0000 |
| 8 | -45.4700 | 36.5600 | 1.0000 |
| 9 | -28.4000 | 53.2200 | 1.0000 |
| 10 | -2.0200 | 63.7200 | 1.0000 |
| 11 | 28.1200 | 63.4400 | 1.0000 |
| 12 | 57.4900 | 52.5500 | 1.0000 |
| 13 | 80.8500 | 34.2000 | 1.0000 |
| 14 | 98.0800 | 9.1400 | 1.0000 |
| 15 | 105.6900 | -17.3000 | 1.0000 |
| 16 | 103.8300 | -46.9600 | 1.0000 |
| 17 | 88.4200 | -71.5000 | 1.0000 |
| 18 | 61.2600 | -86.8400 | 1.0000 |
| 19 | 26.4700 | -91.0700 | 1.0000 |
| 20 | -6.5900 | -81.3700 | 1.0000 |
| 21 | -34.5500 | -59.2400 | 1.0000 |
| 22 | -51.5100 | -29.2800 | 1.0000 |
| 23 | -56.3000 | -2.3100 | 1.0000 |

General Equation of Ellipse with X,Y origin not at centre of ellipse
$a X X+2 h X Y+b Y Y+d X+e Y=1$
$a=1.720717 e-004$
$\mathrm{h}=2.690541 \mathrm{e}-005$
b $=1.865607 e-004$
$d=-7.743828 e-005$
$\mathrm{e}=3.729881 \mathrm{e}-005$
Equation of Ellipse with $x, y$ origin at centre of ellipse
Axx + 2Hxy + Byy = 1
$A=1.535544 \mathrm{e}-004$
H = 2.401002e-005
$B=1.664842 e-004$
Ellipse parameters
semi-major axis a = 86.017
semi-minor axis b $=73.544$
Bearing of major axis
beta(degrees) $=-37.465030$
beta(DMS) = -37 2754.11
Brg (degrees) $=127.465030$
Brg(DMS) $=1272754.11$
Coordinates of centre of ellipse
$X($ centre $)=24.620$
$\mathrm{Y}($ centre $)=\quad-13.547$



Figure 2.8 Plot of Least Squares Best Fit Ellipse and data points for the MCG

The MATLAB program best_fit_ellipse.m calls two other MATLAB functions ellipse.m (a function to compute the coordinates of points on an ellipse) and DMS.m (a function to convert decimal degree to degrees, minutes and seconds). A copy of these programs is shown below.

## MATLAB program best_fit_ellipse

```
function best_fit_ellipse
%
% BEST_FIT_ELLIPSE reads an ASCII textfile containing point numbers of
% coordinate pairs (X,Y) and weights (W) associated with each pair and
% computes the cordinates of the origin, the lengths of the axes and
% the rotation angle of the Best Fit Ellipse using the least squares
% principle. Results are written to a textfile having the same path
% and name as the data file but with the extension ".out"
```

```
%==============================================================================
Function: best_fit_ellipse
%
% Author:
Rod Deakin,
    School of Mathematical and Geospatial Sciences, RMIT University,
    GPO Box 2476V, MELBOURNE VIC 3001
    AUSTRALIA
    email: rod.deakin@rmit.edu.au
    Date:
    Version 1.0 22 March 2003
    Version 1.1 10 May 2003
    Version 1.2 }9\mathrm{ November 2005
    Functions Required:
        [X,Y] = ellipse(a,b,theta)
        [D,M,S] = DMS(DecDeg)
    Remarks:
    The general equation of an ellipse is
        aXX + 2hXY + bYY + dX + eY = 1
    This function computes the parameters a,h,b,d,e of a Least Squares Best Fit
    Ellipse given a set of X,Y coordinate pairs and weights (w) associated with
    each pair. The centre of the best fit ellipse is at Xo = (eh-db)/(2ab-2hh)
    and Yo = (dh-ea)/(2ab-2hh).
    A constant c = 1 - (aXoXo + 2hXoYo + bYoYo + dXo + eYo) is divided into a,
    h and b giving A = a/c, H = h/c and B = b/c which are the parameters of an
    ellipse Axx +2Hxy + Byy = 1. The major axis of this ellipse is rotated
    from the coordinate axes by an angle beta which can be determined from the
    polar equation of an ellipse
    A*cos_squared(theta) + 2H*}\operatorname{cos(theta)*sin(theta) + B*sin_squared(theta) =
/r_squared
    The maximum and minimum values of this function occur for theta given by
    tan(2*theta) = 2H/(A-B) and the angle beta is determined by evaluating
    the sign of the second derivative of the polar equation. This angle is
    substituted into the polar equation to determine the length of the semi-major
    axis length a. Beta - 90 degrees will give the length of the semi-minor
    axis length b
    Note that the semi-axes lengths a,b are not the same as the parameters
    a and b in the general equation of the ellipse.
    Results are written to a textfile having the same path and name as the
    data file but with the extension ".out"
References:
    Notes on Least Squares (2005), Geospatial Science, RMIT
            University, 2005
```


## MATLAB program best_fit_ellipse

```
Arrays:
B - coeff matrix of observation equation v + Bx = f
f - vector of numeric terms
N - coefficient matrix of Normal equations Nx = t
    Ninv - inverse of N
p - vector of perpendicular distances from ellipse to points
point - vector of point numbers
t - vector of numeric terms of Normal equations Nx = t
u,v - vectors of u,v coords of ellipse
W - weight matrix
weight - vector of weights
x - vector of solutions
x,y - vectors of x,y coords of ellipse
x_coord - vector of X coordinates
y_coord - vector of Y coordinates
xpt,ypt - vectors of coords for point number locations on plot
Xpt,Ypt - vectors Xpt = xpt + Xc, Ypt = ypt + Yc
Variables:
A,B,H - parameters of ellipse Axx + 2Hxy + Byy = 1
a,h,b, - parameters of ellipse aXX + 2hXY + bYY + dX + eY = 1
    d,e
a1,b1 - semi-major and semi-minor axes of ellipse
beta - angle between x-axis and major axis of ellipse (degrees)
brg - bearing of major axis (u-axis) of ellipse (degrees)
c - constant of translated ellipse or cos(x)
d2r - degree to radian conversion factor = 180/pi = 57.29577951...
e2 - eccentricity squared
flat - flattening of ellipse
f_dd - second derivative of the function "f" where f is the polar
equation of an ellipse
lat - latitude (radians) of point related to an ellipse
n - number of equations
new_lat - new latitude in iteration
nu - radius of curvature in prime meridian
pion2 - 90 degrees or pi/2
u - number of unknowns
s - sin(x)
s1,s2 - sin(lat) and sin_squared(lat)
scale - scale factor to reduce size of numbers in normal equations
theta - angle for which polar equation of ellipse gives max/min
values
two_theta - 2*theta
Xc,Yc - coords of centre of ellipse X = x + Xc, Y = y + Yc
X0,Y0 - scaled coords of centre of ellipse
```

\%
\% Set program constants
d2r = 180/pi;
pion2 = pi/2;
scale = 100;

## MATLAB program best_fit_ellipse

```
%--------------------------------------------------------------------
% 2. Concatenate strings to give the path and file name of the input file
% 3. Strip off the extension from the file name to give the rootName
% 4. Add extension ".out" to rootName to give the output filename
% 5. Concatenate strings to give the path and file name of the output file
%--------------------------------------------------------------------------
filepath = strcat('c:\temp\','*.dat');
[infilename,inpathname] = uigetfile(filepath);
infilepath = strcat(inpathname,infilename);
rootName = strtok(infilename,'.');
outfilename = strcat(rootName,'.out');
outfilepath = strcat(inpathname,outfilename);
%--------------------------------------------------------
% 1. Load the data into an array whose name is the rootName
% 2. set fileTemp = rootName
% 3. Copy columns of data into individual arrays
%-----------------------------------------------------------
load(infilepath);
fileTemp = eval(rootName);
point = fileTemp(:,1);
x_coord = fileTemp(:,2);
y_coord = fileTemp(:,3);
weight = fileTemp(:,4);
% Determine the number of equations and set the number of unknowns
n = length(point);
u = 5;
% Set the elements of the weight matrix W
W = zeros(n,n);
for k = 1:n
    w(k,k) = weight(k);
end
% Form the coefficient matrix B of the observation equations.
% Note that the coordinates are scaled by a factor 1/100 to
% reduce the size of equations.
B = zeros(n,u);
for k = 1:n
    B}(k,1)=(x_coord(k)/scale)^2
    B(k,2) = (x_coord(k)/scale)*(y_coord(k)/scale);
    B(k,3) = (y_coord(k)/scale)^2;
    B(k,4) = x_coord(k)/scale;
    B(k,5) = y_coord(k)/scale;
end
% Form the vector of numeric terms f
f = ones(n,1);
% Form the normal equation coefficient matrix N
% and the vector of numeric terms t
N = B'*W*B;
t = B'*W*f;
% Compute the inverse and solve the system Nx = t
Ninv = inv(N);
x = Ninv*t;
```


## MATLAB program best_fit_ellipse

```
% Copy the results into the variables a,h,b,d,e
a = x(1,1);
h = x(2,1)/2;
b = x(3,1);
d = x (4,1);
e = x(5,1);
% Compute the coordinates of the centre of the ellipse
X0 = (e*h - b*d)/(2*(a*b - h*h));
Y0 = (d*h - a*e)/(2*(a*b - h*h));
Xc = X0*scale;
Yc = Y0*scale;
% Compute the variables A,H,B and then the lengths
% of the axes and the rotation angle beta
c = 1-(a*X0*X0 + 2*h*X0*Y0 + b*Y0*Y0 + d*X0 + e*Y0);
A = a/c
H = h/c;
B = b/c
% compute the angle theta for max or min
two_theta = atan2(2*H,(A-B));
% compute second derivative
f_dd = 2*(B-A)*cos(two_theta) - 4*H*sin(two_theta);
% test the second derivative to determine max or min
theta = two_theta/2;
if f_dd < 0
    beta = theta - pion2;
else
    beta = theta;
end
% compute semi-major axis length
c = cos(beta);
s = sin(beta);
a1 = sqrt(1/(A*C*c + 2*H*C*s + B*s*s))*scale;
% compute semi-minor axis length
c = cos(beta+pion2);
s = sin(beta+pion2);
b1 = sqrt(1/(A*c*c + 2*H*c*s + B*s*s))*scale;
% convert beta to degrees
beta = beta*d2r;
% Calculate bearing of major axis noting that the rotation angle
% beta is considered positive anti-clockwise from the X-axis to
% the major axis of the ellipse
brg = 360+90-beta;
if(brg>360)
    brg = brg-360;
end
%------------------------------------------------------------------------
% Compute perpendicular distances from points to the ellipse of best fit
%------------------------------------------------------------------------
% Create a set of u,v coordinates by first reducing the X,Y coords
% to x,y coordinates and then rotating these coordinates by the
% rotation angle beta. The u-axis is the major axis of the ellipse.
x = x_coord-Xc;
y = y_coord-Yc;
for k=1:n
    u(k,1) = x(k)*cos(beta/d2r) + y(k)*sin(beta/d2r);
    v(k,1) = -x(k)*sin(beta/d2r) + y(k)*cos(beta/d2r);
end
```


## MATLAB program best_fit_ellipse

```
% Compute the flattening and eccentricity squared for the ellipse
flat = (a1-b1)/a1;
```

e2 = flat*(2-flat);
\% Compute the distance along the normal to the ellipse passing
\% through the point
for $k=1$ : $n$
\% Compute the latitude of the normal to the ellipse through
$\%$ the point by iteration. nu is the radius of curvature of
\% the prime vertical normal section
lat $=\mathrm{pi} / 2$;
new_lat $=\operatorname{atan2}(v(k, 1), u(k, 1))$;
while(abs(new_lat-lat)>1e-10)
lat = new_lat;
s1 $=\sin ($ lat $)$;
s2 = s1*s1;
nu = a1/sqrt(1-e2*s2);
new_lat $=$ atan2((v(k,1)+nu*e2*s1), $u(k, 1))$;
end
$\% \mathrm{p}$ is the distance along the normal from the ellipse to the point
$p(k, 1)=(u(k, 1) / \cos (l a t))-n u$;
end
\%--------------------------------------------------
\% Compute the coordinate locations for a point number
\% to be shown on the plot. These locations used in
\% in the plot routines below.
\%-------
theta $=\operatorname{atan} 2(x(k), y(k))$;
if theta<0
theta $=$ theta $+2 *$ pi;
end
$r=\operatorname{sqrt}\left(x(k)^{\wedge} 2+y(k)^{\wedge} 2\right)-10$;
xpt(k) $=r^{*} \sin ($ theta $)$;
ypt(k) $=r^{*} \cos ($ theta $)$;
end
Xpt $=x p t+X c ;$
Ypt = ypt + Yc;
\%-----------------------------
\% print the data to the screen
\%----------------------------
fprintf('\n Ellipse of Best Fit\n');
fprintf('\n General Equation of Ellipse with $X, Y$ origin not at centre of ellipse');
fprintf('\n aXX + 2hXY + bYY + dX + eY = 1');
fprintf('\n a = \%14.6e',a/scale^2);
fprintf('\n h = \%14.6e',h/scale^2);
fprintf('\n b = \%14.6e',b/scale^2);
fprintf('\n d = \%14.6e',d/scale^2);
fprintf('\n e = \%14.6e\n',e/scale^2);
fprintf('\n Equation of Ellipse with $x, y$ origin at centre of ellipse');
fprintf('\n Axx + 2Hxy + Byy = 1');
fprintf('\n A = \%14.6e', A/scale^2)';
fprintf('\n H = \%14.6e', H/scale^2);
fprintf('\n B = \%14.6e\n',B/scale^2);
fprintf('\n Ellipse parameters');
fprintf('\n semi-major axis a = \%8.3f', a1);
fprintf('\n semi-minor axis b = \%8.3f\n',b1);
fprintf('\n Bearing of major axis');
fprintf('\n beta(degrees) $=\% 12.6 f^{\prime}$, beta);
[D, M, S] = DMS(beta);
fprintf('\n beta(DMS) = \%4d \%2d \%5.2f',D,M,S);
fprintf('\n Brg(degrees) = \%12.6f',brg);

## MATLAB program best_fit_ellipse

```
[D,M,S] = DMS(brg);
fprintf('\n Brg(DMS) = %4d %2d %5.2f\n',D,M,S);
fprintf('\n Coordinates of centre of ellipse');
fprintf('\n X(centre) = %12.3f',Xc);
fprintf('\n Y(centre) = %12.3f\n',Yc);
fprintf('\n Data and offsets to ellipse of best fit');
fprintf('\n pt offset X Y X
v');
for k=1:n
    fprintf('\n %3d %10.3f %10.3f %10.3f %10.3f %10.3f %10.3f
%10.3f', point(k),p(k,1),x_coord(k),y_coord(k),x(k),y(k),u(k,1),v(k,1));
end
fprintf('\n\n');
%--------------------------------
% print the data to the output file
%----------------------------------
% Open the output file
fidout = fopen(outfilepath,'wt');
fprintf(fidout,'\n\nEllipse of Best Fit Least Squares Solution');
fprintf(fidout,'\n\nInput Data');
fprintf(fidout,'\n point x(k) y(k) weight w(k)');
for k = 1:n
    fprintf(fidout,'\n%3d %12.4f %12.4f
%12.4f',point(k),x_coord(k),y_coord(k),weight(k));
end
fprintf(fidout,'\n\n General Equation of Ellipse with X,Y origin not at centre of
ellipse');
fprintf(fidout,'\n aXX + 2hXY + bYY + dX + eY = 1');
fprintf(fidout,'\n a = %14.6e',a/scale^2);
fprintf(fidout,'\n h = %14.6e',h/scale^2);
fprintf(fidout,'\n b = %14.6e',b/scale^2);
fprintf(fidout,'\n d = %14.6e',d/scale^2);
fprintf(fidout,'\n e = %14.6e\n',e/scale^2);
fprintf(fidout,'\n Equation of Ellipse with x,y origin at centre of ellipse');
fprintf(fidout,'\n Axx + 2Hxy + Byy = 1');
fprintf(fidout,'\n A = %14.6e',A/scale^2);
fprintf(fidout,'\n H = %14.6e',H/scale^2);
fprintf(fidout,'\n B = %14.6e\n',B/scale^2);
fprintf(fidout,'\n Ellipse parameters');
fprintf(fidout,'\n semi-major axis a = %8.3f',a1);
fprintf(fidout,'\n semi-minor axis b = %8.3f\n',b1);
fprintf(fidout,'\n Bearing of major axis');
fprintf(fidout,'\n beta(degrees) = %12.6f',beta);
[D,M,S] = DMS(beta);
fprintf(fidout,'\n beta(DMS) = %4d %2d %5.2f',D,M,S);
fprintf(fidout,'\n Brg(degrees) = %12.6f',brg);
[D,M,S] = DMS(brg);
fprintf(fidout,'\n Brg(DMS) = %4d %2d %5.2f\n',D,M,S);
fprintf(fidout,'\n Coordinates of centre of ellipse');
fprintf(fidout,'\n X(centre) = %12.3f',Xc);
fprintf(fidout,'\n Y(centre) = %12.3f\n',Yc);
fprintf(fidout,'\n Data and offsets to ellipse of best fit');
fprintf(fidout,'\n pt offset X Y y 
u v');
for k=1:n
    fprintf(fidout,'\n %3d %10.3f %10.3f %10.3f %10.3f %10.3f %10.3f
%10.3f',point(k),p(k,1),x_coord(k),y_coord(k),x(k),y(k),u(k,1),v(k,1));
end
```

```
                                    MATLAB program best_fit_ellipse
fprintf(fidout,'\n\n');
% Close the output file
fclose(fidout);
%------------------------------------------------------------------
% Call function 'ellipse' with parameters a,b,theta and receive back
% X,Y coordinates whose origin is at the centre of the ellipse
%-------------------------------------------------------------------
[X,Y] = ellipse(a1,b1,beta);
X = X + Xc;
Y = Y + Yc;
%-------------------------------------------------------------------
% Set the X,Y coordinates of the major and minor axes of the ellipse
%--------------------------------------------------------------------
aX = [X(180) X(360)];
aY = [Y(180) Y(360)];
bX = [X(90) X(270)];
bY = [Y(90) Y(270)];
%-----------------------------------------------
% plot the ellipse of Best Fit and the data points
%-------------------------------------------------
figure(1);
clf(1);
plot(X,Y,'r-',aX,aY,'b-',bX,bY,'b-');
hold on;
plot(x_coord,y_coord,'k.');
axis equal;
box off;
% plot the point numbers inside the ellipse
point_string=int2str(point);
text(Xpt,Ypt,point_string);
% anotate the plot
title('Least Squares Ellipse of Best Fit')
xlabel('X coordinate');
ylabel('Y coordinate');
```


## MATLAB program ellipse

```
function [X,Y] = ellipse(a,b,theta)
% ELLIPSE[X Y] = (A,B,THETA) Function to compute the X,Y coordinates of
% an ellipse given semi-axes A and B and a rotation angle THETA.
% The angle THETA is considered to be positive anti-clockwise from the x-axis
% set degree to radian conversion factor
d2r = pi/180;
% Calculate u,v coordinates of ellipse using parametric equations
% u = a*cos(psi)
% v = b*sin(psi)
% where the u-axis is the major axis, the v-axis is the minor axis
% and psi is the auxiliary angle measured positive anti-clockwise
% from the u-axis to a point moving around the auxiliary circle of
% radius a. The x,y coordinates are computed by rotating the ellipse
% axes by an angle theta, considered as positive anti-clockwise from the x-axis.
% x = u*cos(theta) - v*sin(theta)
% y = u*sin(theta) + v* cos(theta)
for k=1:360
    u = a*cos(k*d2r);
    v = b*sin(k*d2r);
    X(k) = u*cos(theta*d2r) - v*sin(theta*d2r);
    Y(k) = u*sin(theta*d2r) + v*cos(theta*d2r);
end
return
```


## MATLAB program DMS

```
function [D,M,S] = DMS(DecDeg)
% [D,M,S] = DMS(DecDeg) This function takes an angle in decimal degrees
% and returns Degrees, Minutes and Seconds
val = abs(DecDeg);
D = fix(val);
M = fix((val-D)*60);
S = (val-D-M/60)*3600;
if(DecDeg<0)
    D = -D;
end
return
```

