5. PROPAGATION OF VARIANCES APPLIED TO LEAST SQUARES ADJUSTMENT OF INDIRECT OBSERVATIONS

A most important outcome of a least squares adjustment is that estimates of the precisions of the quantities sought, the elements of **x**, the unknowns or the parameters, are easily obtained from the matrix equations of the solution. Application of the Law of Propagation of Variances demonstrates that $\mathbf{N}^{-1}$, the inverse of the normal equation coefficient matrix is equal to the cofactor matrix $\mathbf{Q}_{xx}$ that contains estimates of the variances and covariances of the elements of **x**. In addition, estimates of the precisions of the residuals and adjusted observations may be obtained. This most useful outcome enables a statistical analysis of the results of a least squares adjustment and provides the practitioner with a degree of confidence in the results.

5.1. Cofactor matrices for adjustment of indirect observations

The observation equations for adjustment of indirect observations is given by

$$\mathbf{v} + \mathbf{B}\mathbf{x} = \mathbf{f} \tag{5.1}$$

f is an $(n,1)$ vector of numeric terms derived from the $(n,1)$ vector of observations **l** and the $(n,1)$ vector of constants **d** as

$$\mathbf{f} = \mathbf{d} - \mathbf{l} \tag{5.2}$$

Associated with the vector of observations **l** is a variance-covariance matrix Σ_{ll} as well as a cofactor matrix $\mathbf{Q}_{ll}$ and a weight matrix $\mathbf{W}_{ll} = \mathbf{Q}_{ll}^{-1}$. Remember that in most practical applications of least squares, the matrix Σ_{ll} is unknown, <u>but</u> estimated *a priori* by $\mathbf{Q}_{ll}$ that contains estimates of the variances and covariances and $\mathbf{\Sigma}_{ll} = \sigma_0^2 \mathbf{Q}_{ll}$ where σ_0^2 is the reference variance or variance factor.

Note: In the derivations that follow, the subscript *"ll"* is dropped from $\mathbf{Q}_{ll}$ and $\mathbf{W}_{ll}$

If equation (5.2) is written as

$$\mathbf{f} = (-\mathbf{I})\mathbf{l} + \mathbf{d} \tag{5.3}$$

then (5.3) is in a form suitable for employing the Law of Propagation of Variances developed in Chapter 3; i.e., if $\mathbf{y} = \mathbf{A}\mathbf{x} + \mathbf{b}$ and **y** and **x** are random variables linearly related and **b** is a vector of constants then $\mathbf{Q}_{yy} = \mathbf{A}\mathbf{Q}_{xx}\mathbf{A}^T$. Hence, the cofactor matrix of the numeric terms **f** is

$$\mathbf{Q}_{ff} = (-\mathbf{I})\mathbf{Q}(-\mathbf{I})^T = \mathbf{Q}$$

Thus the cofactor matrix of **f** is also the *a priori* cofactor matrix of the observations **l**.

The solution "steps" in the least squares adjustment of indirect observations are set out Chapter 2 and restated as

$$\begin{aligned} \mathbf{N} &= \mathbf{B}^T\mathbf{W}\mathbf{B} \\ \mathbf{t} &= \mathbf{B}^T\mathbf{W}\mathbf{f} \\ \mathbf{x} &= \mathbf{N}^{-1}\mathbf{t} \\ \mathbf{v} &= \mathbf{f} - \mathbf{B}\mathbf{x} \\ \hat{\mathbf{l}} &= \mathbf{l} + \mathbf{v} \end{aligned}$$

To apply the Law of Propagation of Variances, these equations may be re-arranged in the form $\mathbf{y} = \mathbf{A}\mathbf{x} + \mathbf{b}$ where the terms in parenthesis ( ) constitute the **A** matrix.

$$\mathbf{t} = \left(\mathbf{B}^T\mathbf{W}\right)\mathbf{f} \tag{5.4}$$

$$\mathbf{x} = \left(\mathbf{N}^{-1}\right)\mathbf{t} \tag{5.5}$$

$$\begin{aligned} \mathbf{v} &= \mathbf{f} - \mathbf{B}\mathbf{x} \\ &= \mathbf{f} - \mathbf{B}\mathbf{N}^{-1}\mathbf{t} \\ &= \mathbf{f} - \mathbf{B}\mathbf{N}^{-1}\mathbf{B}^T\mathbf{W}\mathbf{f} \\ &= \left(\mathbf{I} - \mathbf{B}\mathbf{N}^{-1}\mathbf{B}^T\mathbf{W}\right)\mathbf{f} \end{aligned} \tag{5.6}$$

$$\begin{aligned} \hat{\mathbf{l}} &= \mathbf{l} + \mathbf{v} \\ &= \mathbf{l} + \mathbf{f} - \mathbf{B}\mathbf{x} \\ &= \mathbf{d} - \mathbf{B}\mathbf{x} \\ &= (-\mathbf{B})\mathbf{x} + \mathbf{d} \end{aligned} \tag{5.7}$$

Applying the Law of Propagation of Variances to equations (5.4) to (5.7) gives the following cofactor matrices

$$\mathbf{Q}_{tt} = \left(\mathbf{B}^T\mathbf{W}\right)\mathbf{Q}_{ff}\left(\mathbf{B}^T\mathbf{W}\right)^T = \mathbf{N} \tag{5.8}$$

$$\mathbf{Q}_{xx} = \left(\mathbf{N}^{-1}\right)\mathbf{Q}_{tt}\left(\mathbf{N}^{-1}\right)^T = \mathbf{N}^{-1} \tag{5.9}$$

$$\begin{aligned}\mathbf{Q}_{vv} &= \left(\mathbf{I}-\mathbf{B}\mathbf{N}^{-1}\mathbf{B}^T\mathbf{W}\right)\mathbf{Q}_{ff}\left(\mathbf{I}-\mathbf{B}\mathbf{N}^{-1}\mathbf{B}^T\mathbf{W}\right)^T \\ &= \mathbf{Q}-\mathbf{B}\mathbf{N}^{-1}\mathbf{B}^T\end{aligned} \tag{5.10}$$

$$\begin{aligned}\mathbf{Q}_{\hat{l}\hat{l}} &= \left(-\mathbf{B}\right)\mathbf{Q}\left(-\mathbf{B}\right)^T \\ &= \mathbf{B}\mathbf{N}^{-1}\mathbf{B}^T \\ &= \mathbf{Q}-\mathbf{Q}_{vv}\end{aligned} \tag{5.11}$$

Variance-covariance matrices for $\mathbf{t}$, $\mathbf{x}$, $\mathbf{v}$ and $\hat{\mathbf{l}}$ are obtained by multiplying the cofactor matrix by the variance factor σ_0^2.

5.2. Calculation of the quadratic form $\mathbf{v}^T\mathbf{W}\mathbf{v}$

The *a priori* estimate of the variance factor may be computed from

$$\hat{\sigma}_0^2 = \frac{\mathbf{v}^T\mathbf{W}\mathbf{v}}{r} \tag{5.12}$$

where $\mathbf{v}^T\mathbf{W}\mathbf{v}$ is the quadratic form, and

$r = n - u$ is the degrees of freedom where n is the number of observations and u is the number of unknown parameters. r is also known as the number of redundancies.

A derivation of equation (5.12) is given below. The quadratic form $\mathbf{v}^T\mathbf{W}\mathbf{v}$ may be computed in the following manner.

Remembering, for the method of indirect observations, the following matrix equations

$$\begin{aligned}\mathbf{N} &= \mathbf{B}^T\mathbf{W}\mathbf{B} \\ \mathbf{t} &= \mathbf{B}^T\mathbf{W}\mathbf{f} \\ \mathbf{x} &= \mathbf{N}^{-1}\mathbf{t} \\ \mathbf{v} &= \mathbf{f}-\mathbf{B}\mathbf{x}\end{aligned}$$

then

$$\begin{aligned}\mathbf{v}^T\mathbf{W}\mathbf{v} &= (\mathbf{f}-\mathbf{B}\mathbf{x})^T\mathbf{W}(\mathbf{f}-\mathbf{B}\mathbf{x})\\ &= (\mathbf{f}^T-\mathbf{x}^T\mathbf{B}^T)\mathbf{W}(\mathbf{f}-\mathbf{B}\mathbf{x})\\ &= (\mathbf{f}^T\mathbf{W}-\mathbf{x}^T\mathbf{B}^T\mathbf{W})(\mathbf{f}-\mathbf{B}\mathbf{x})\\ &= \mathbf{f}^T\mathbf{W}\mathbf{f}-\mathbf{f}^T\mathbf{W}\mathbf{B}\mathbf{x}-\mathbf{x}^T\mathbf{B}^T\mathbf{W}\mathbf{f}+\mathbf{x}^T\mathbf{B}^T\mathbf{W}\mathbf{B}\mathbf{x}\\ &= \mathbf{f}^T\mathbf{W}\mathbf{f}-2\mathbf{f}^T\mathbf{W}\mathbf{B}\mathbf{x}+\mathbf{x}^T\mathbf{B}^T\mathbf{W}\mathbf{B}\mathbf{x}\\ &= \mathbf{f}^T\mathbf{W}\mathbf{f}-2\mathbf{t}^T\mathbf{x}+\mathbf{x}^T\mathbf{N}\mathbf{x}\\ &= \mathbf{f}^T\mathbf{W}\mathbf{f}-2\mathbf{x}^T\mathbf{t}+\mathbf{x}^T\mathbf{t}\end{aligned}$$

and

$$\mathbf{v}^T\mathbf{W}\mathbf{v} = \mathbf{f}^T\mathbf{W}\mathbf{f}-\mathbf{x}^T\mathbf{t} \tag{5.13}$$

5.3. Calculation of the Estimate of the Variance Factor $\hat{\sigma}_0^2$

The variance-covariance matrices of residuals $\mathbf{\Sigma}_{vv}$, adjusted observations $\mathbf{\Sigma}_{\hat{l}\hat{l}}$ and computed parameters $\mathbf{\Sigma}_{xx}$ are calculated from the general relationship

$$\mathbf{\Sigma} = \sigma_0^2\mathbf{Q} \tag{5.14}$$

Cofactor matrices $\mathbf{Q}_{vv}$, $\mathbf{Q}_{xx}$ and $\mathbf{Q}_{\hat{l}\hat{l}}$ are computed from equations (5.9) to (5.11) and so it remains to determine an estimate of the variance factor $\hat{\sigma}_0^2$.

The development of a matrix expression for computing $\hat{\sigma}_0^2$ is set out below and follows Mikhail (1976, pp.285-288). Some preliminary relationships will be useful.

1. If **A** is an (n,n) square matrix, the sum of its diagonal elements is a scalar quantity called the trace of **A** and denoted by $tr(\mathbf{A})$ The following relationships are useful

$$tr(\mathbf{A}+\mathbf{B}) = tr(\mathbf{A})+tr(\mathbf{B}) \quad \text{for } \mathbf{A} \text{ and } \mathbf{B} \text{ of same order} \tag{5.15}$$

$$tr(\mathbf{A}^T) = tr(\mathbf{A}) \tag{5.16}$$

and for the quadratic form $\mathbf{x}^T\mathbf{A}\mathbf{x}$ where **A** is symmetric

$$\mathbf{x}^T\mathbf{A}\mathbf{x} = tr(\mathbf{x}\mathbf{x}^T\mathbf{A}) \tag{5.17}$$

2. The variance-covariance matrix $\boldsymbol{\Sigma}_{xx}$ given by equation (3.21) can be expressed in the following manner, remembering that **x** is a vector of <u>random variables</u> and $\mathbf{m}_x$ is a vector of <u>means</u>.

$$\begin{aligned}\Sigma_{xx} &= E\left\{(\mathbf{x}-\mathbf{m}_x)(\mathbf{x}-\mathbf{m}_x)^T\right\}\\ &= E\left\{(\mathbf{x}-\mathbf{m}_x)(\mathbf{x}^T-\mathbf{m}_x^T)\right\}\\ &= E\left\{\mathbf{x}\mathbf{x}^T-\mathbf{x}\mathbf{m}_x^T-\mathbf{m}_x\mathbf{x}^T+\mathbf{m}_x\mathbf{m}_x^T\right\}\\ &= E\left\{\mathbf{x}\mathbf{x}^T\right\}-E\left\{\mathbf{x}\mathbf{m}_x^T\right\}-E\left\{\mathbf{m}_x\mathbf{x}^T\right\}+E\left\{\mathbf{m}_x\mathbf{m}_x^T\right\}\\ &= E\left\{\mathbf{x}\mathbf{x}^T\right\}-E\left\{\mathbf{x}\right\}\mathbf{m}_x^T-\mathbf{m}_xE\left\{\mathbf{x}^T\right\}+\mathbf{m}_x\mathbf{m}_x^T\end{aligned}$$

Now from equation (3.18) $\mathbf{m}_x = E\left\{\mathbf{x}\right\}$ hence

$$\begin{aligned}\Sigma_{xx} &= E\left\{\mathbf{x}\mathbf{x}^T\right\}-\mathbf{m}_x\mathbf{m}_x^T-\mathbf{m}_x\mathbf{m}_x^T+\mathbf{m}_x\mathbf{m}_x^T\\ &= E\left\{\mathbf{x}\mathbf{x}^T\right\}-\mathbf{m}_x\mathbf{m}_x^T \qquad (5.18)\end{aligned}$$

or

$$E\left\{\mathbf{x}\mathbf{x}^T\right\} = \boldsymbol{\Sigma}_{xx}+\mathbf{m}_x\mathbf{m}_x^T \qquad (5.19)$$

3. The expected value of the residuals is zero, i.e.,

$$E\left\{\mathbf{v}\right\} = \mathbf{m}_v = \mathbf{0} \qquad (5.20)$$

4. By definition (see Chapter 2) the weight matrix **W**, the cofactor matrix **Q** and the variance-covariance matrix $\boldsymbol{\Sigma}$ are related by

$$\mathbf{W} = \mathbf{Q}^{-1} = \sigma_0^2\boldsymbol{\Sigma}^{-1} \qquad (5.21)$$

Now, for the least squares adjustment of indirect observations the following relationships are recalled

$$\mathbf{v}+\mathbf{B}\mathbf{x} = \mathbf{f}, \quad \mathbf{N} = \mathbf{B}^T\mathbf{W}\mathbf{B}, \quad \mathbf{t} = \mathbf{B}^T\mathbf{W}\mathbf{f}$$
$$\mathbf{Q}_{ff} = \mathbf{Q}, \quad \mathbf{Q}_{tt} = \mathbf{N}, \quad \mathbf{Q}_{xx} = \mathbf{N}^{-1}$$

Bearing in mind equation (5.21), the following relationships may be introduced

$$\boldsymbol{\Sigma}^{-1} = \frac{1}{\sigma_0^2}\mathbf{W}, \quad \mathbf{M} = \mathbf{B}^T\boldsymbol{\Sigma}^{-1}\mathbf{B}$$

and from these follow

$$\Sigma_{ff} = \mathbf{\Sigma}, \quad \Sigma_{tt} = \sigma_0^4 \mathbf{M}, \quad \Sigma_{xx} = \mathbf{M}^{-1}$$

In addition, the expectation of the vector **f** is the mean $\mathbf{m}_f$ and so we may write

$$\mathbf{m}_f = E\{\mathbf{f}\} = E\{\mathbf{v} + \mathbf{Bx}\} = E\{\mathbf{v}\} + \mathbf{B}\, E\{\mathbf{x}\}$$

Now since $E\{\mathbf{x}\} = \mathbf{m}_x$ and $E\{\mathbf{v}\} = \mathbf{0}$

$$\mathbf{m}_f = \mathbf{Bm}_x \tag{5.22}$$

Now the quadratic form

$$\mathbf{v}^T \mathbf{Wv} = \sigma_0^2 \left(\mathbf{v}^T \mathbf{\Sigma}^{-1} \mathbf{v} \right) \tag{5.23}$$

and from equation (5.13)

$$\begin{aligned} \mathbf{v}^T \mathbf{Wv} &= \mathbf{f}^T \mathbf{Wf} - \mathbf{x}^T \mathbf{t} \\ &= \mathbf{f}^T \mathbf{Wf} - \mathbf{x}^T \mathbf{Nx} \end{aligned}$$

Using the relationships above

$$\mathbf{v}^T \mathbf{\Sigma}^{-1} \mathbf{v} = \mathbf{f}^T \mathbf{\Sigma}^{-1} \mathbf{f} - \mathbf{x}^T \mathbf{Mx}$$

Now the expected value of this quadratic form is

$$\begin{aligned} E\left\{\mathbf{v}^T \mathbf{\Sigma}^{-1} \mathbf{v}\right\} &= E\left\{\mathbf{f}^T \mathbf{\Sigma}^{-1} \mathbf{f} - \mathbf{x}^T \mathbf{Mx}\right\} \\ &= E\left\{\mathbf{f}^T \mathbf{\Sigma}^{-1} \mathbf{f}\right\} - E\left\{\mathbf{x}^T \mathbf{Mx}\right\} \end{aligned}$$

Recognising that the terms on the right-hand-side are both quadratic forms, equation (5.17) can be used to give

$$\begin{aligned} E\left\{\mathbf{v}^T \mathbf{\Sigma}^{-1} \mathbf{v}\right\} &= E\left\{tr\left(\mathbf{ff}^T \mathbf{\Sigma}^{-1}\right)\right\} - E\left\{tr\left(\mathbf{xx}^T \mathbf{M}\right)\right\} \\ &= tr\left(E\left\{\mathbf{ff}^T \mathbf{\Sigma}^{-1}\right\}\right) - tr\left(E\left\{\mathbf{xx}^T \mathbf{M}\right\}\right) \\ &= tr\left(E\left\{\mathbf{ff}^T\right\} \mathbf{\Sigma}^{-1}\right) - tr\left(E\left\{\mathbf{xx}^T\right\} \mathbf{M}\right) \end{aligned}$$

Now using equation (5.19)

$$\begin{aligned} E\left\{\mathbf{v}^T \mathbf{\Sigma}^{-1} \mathbf{v}\right\} &= tr\left(\left[\mathbf{\Sigma}_{ff} + \mathbf{m}_f \mathbf{m}_f^T\right] \mathbf{\Sigma}^{-1}\right) - tr\left(\left[\mathbf{\Sigma}_{xx} + \mathbf{m}_x \mathbf{m}_x^T\right] \mathbf{M}\right) \\ &= tr\left(\mathbf{I}_{nn} + \mathbf{m}_f \mathbf{m}_f^T \mathbf{\Sigma}^{-1}\right) - tr\left(\mathbf{I}_{uu} + \mathbf{m}_x \mathbf{m}_x^T \mathbf{M}\right) \\ &= tr\left(\mathbf{I}_{nn} - \mathbf{I}_{uu}\right) - tr\left(\mathbf{m}_f \mathbf{m}_f^T \mathbf{\Sigma}^{-1} + \mathbf{m}_x \mathbf{m}_x^T \mathbf{M}\right) \\ &= (n - u) - \mathbf{m}_f^T \mathbf{\Sigma}^{-1} \mathbf{m}_f + \mathbf{m}_x^T \mathbf{Mm}_x \end{aligned}$$

From equation (5.22) $\mathbf{m}_f = \mathbf{B}\mathbf{m}_x$ hence using the rule for matrix transpose $\mathbf{m}_f^T = \left(\mathbf{B}\mathbf{m}_x\right)^T = \mathbf{m}_x^T\mathbf{B}^T$, then

$$\begin{aligned} E\left\{\mathbf{v}^T\mathbf{\Sigma}^{-1}\mathbf{v}\right\} &= (n-u) - \mathbf{m}_x^T\mathbf{B}^T\mathbf{\Sigma}^{-1}\mathbf{B}\mathbf{m}_x + \mathbf{m}_x^T\mathbf{M}\mathbf{m}_x \\ &= (n-u) - \mathbf{m}_x^T\mathbf{M}\mathbf{m}_x + \mathbf{m}_x^T\mathbf{M}\mathbf{m}_x \\ &= (n-u) \end{aligned}$$

Thus according to equation (5.23) and the expression above

$$\begin{aligned} E\left\{\mathbf{v}^T\mathbf{W}\mathbf{v}\right\} &= \sigma_0^2 E\left\{\mathbf{v}^T\mathbf{\Sigma}^{-1}\mathbf{v}\right\} \\ &= \sigma_0^2 (n-u) \end{aligned}$$

from which follows

$$\sigma_0^2 = \frac{E\left\{\mathbf{v}^T\mathbf{W}\mathbf{v}\right\}}{n-u}$$

Consequently, an unbiased estimate of the variance factor $\hat{\sigma}_0^2$ can be computed from

$$\hat{\sigma}_0^2 = \frac{\mathbf{v}^T\mathbf{W}\mathbf{v}}{n-u} = \frac{\mathbf{v}^T\mathbf{W}\mathbf{v}}{r} \tag{5.24}$$

$r = n - u$ is the number of redundancies in the adjustment and is known as the degrees of freedom

Using equation (5.13) an unbiased estimate of the variance factor $\hat{\sigma}_0^2$ can be computed from

$$\hat{\sigma}_0^2 = \frac{\mathbf{f}^T\mathbf{W}\mathbf{f} - \mathbf{x}^T\mathbf{t}}{r} \tag{5.25}$$