LEAST SQUARES ADJUSTMENT
A MODERN APPROACH

by

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Part C: CONFIDENCE REGIONS AND TESTS OF LINEAR HYPOTHESES

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Preface

For his lectures at the Tongji University in Shanghai and at other institutions in China in November - December 1981, Peter Meissl prepared a set of lecture notes on contemporary least-squares adjustment and applications. Subsequently he worked on correcting and expanding them, but this was interrupted by his tragic death on May 22, 1982. (For Peter Meissl's life and work, the reader is referred to his biography by Franz Allmer, Mitteilungen der geodätischen Institute der Technischen Universität Graz, Folge 44, 1983.)

In view of the unique importance of this work, the Institute of Theoretical Geodesy decided to edit the manuscript posthumously and to publish the book in the series of the Geodetic Institutes of the Technical University, Graz, although Peter Meissl himself would certainly have included additional topics such as inner adjustment theory, expanded others such as the theory of large networks, and polished the manuscript much more before being satisfied with its publication.

The finishing of the book is due to Peter Meissl's closest associates: Dr. Norbert Bartelme, Dr. Helmut Fuchs, Dr. Bernhard Hofmann-Wellenhof, Dipl.-Ing. Wolf-Dieter Schuh and Dipl.-Ing. Manfred Wieser. In addition to being responsible for the careful editing of the manuscript, they also prepared the printing text using the word processing facilities of the computer WANG 2200 MVP.

A glance at the table of contents shows that this book is a thoroughly modern text on least-squares adjustment. In the contemporary spirit, the usual linear algebra is treated in the context of general linear spaces, which makes possible an easy transition to Hilbert space important for advanced topics. Also modern is the division into an algebraic and geometric approach (without statistics) and a stochastic approach, including statistical tests. Applications to Doppler observations, large networks, geodetic data bases, and splines essentially increase the practical usefulness. Although the book develops adjustment theory in a systematic and self-contained way, it will be best appreciated by readers who already have some elementary previous knowledge of adjustment computations.

The book needs no recommendation. Both students and research workers will find it indispensable. It is a fitting memorial of a great scientist.

Helmut Moritz

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C. CONFIDENCE REGIONS AND TESTS OF LINEAR HYPOTHESES.

1. Probability distributions used in statistical tests.

1.1. One dimensional Gauss distribution (normal distribution).

Let X be a one- dimensional random variable having the probability density

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left|- \frac{(x-\mu)^2}{2\sigma^2}\right|$$

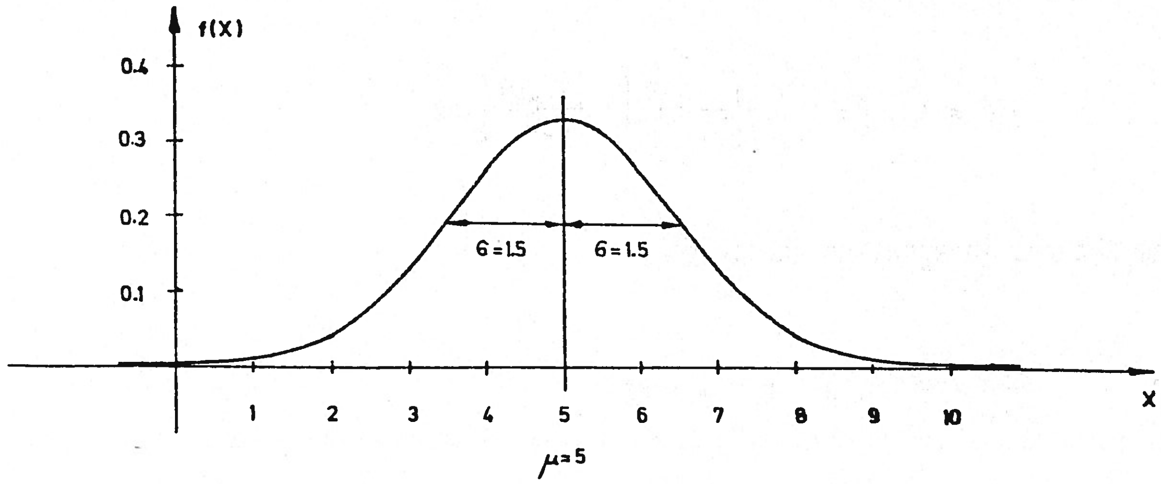
One can prove that

$$E(X) = \int_{-\infty}^{+\infty} x\ f(x)\ dx = \mu$$

$$\sigma^2(X) = \int_{-\infty}^{+\infty} (x-\mu)^2\ f(x)\ dx = \sigma^2$$

Hence μ is the expectation or mean value of X, σ^2 is its variance. The square root of σ^2 is denoted σ. It is called standard deviation.

The graph of f(x) is bell- shaped:



Remark: It is frequently assumed that observation errors are normally distributed. There is no completely rigorous justification for this assumption. However strong support comes from the central limit theorem of probability theory. It can be shown that the sum of a large number of small random variables has a tendency to be normally distributed. This holds under fairly general assumptions. The small elementary random effects may be arbitrarily distributed.

Important special case: The normalized Gauss distribution. It relies on the special choice

$$\mu = 0, \ \sigma = 1$$

consequently

$$f(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right)$$

All tabulations of the Gauss distribution refer to the normalized case. That this is completely sufficient is demonstrated by the following example. Suppose that the Gauss distribution under consideration is not normalized, and suppose that one wishes to calculate the probability of $\alpha \leq X \leq \beta$

$$p\{\alpha \leq X \leq \beta\} = \int_{\alpha}^{\beta} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) dx$$

One changes integration variables

$$\frac{x-\mu}{\sigma} = \xi, \quad \text{i.e.} \quad x = \mu + \sigma\xi$$

One obtains

$$p\{\alpha \leq x \leq \beta\} = \int_{(\alpha-\mu)/\sigma}^{(\beta-\mu)/\sigma} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\xi^2}{2}\right) d\xi$$

It is seen that one calculates the probability

$$p\left\{\frac{\alpha-\mu}{\sigma} \leq \Xi \leq \frac{\beta-\mu}{\sigma}\right\}$$

thereby Ξ has the normalized Gauss distribution. In tabulation one usually finds values of the distribution function

$$F(x) = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{\xi^2}{2}\right) d\xi$$

Hence

$$p\{\alpha \leq X \leq \beta\} = F\left(\frac{\beta-\mu}{\sigma}\right) - F\left(\frac{\alpha-\mu}{\sigma}\right)$$

Remark: The probability of the event

$$-k\sigma \leq X-\mu \leq +k\sigma$$

depends on k only. It equals the probability of

$$-k \leq \Xi \leq +k$$

where Ξ has the normalized Gauss distribution.

Usually one focuses interest on the complementary event, i.e.

$$|X-\mu| > k\sigma$$

The probability of $X-\mu$ exceeding the $k\sigma$- limits is small for moderately large k. For k=3 one obtains

$$p\{|X-\mu| > 3\sigma\} = 0.0027$$

This is about 3 parts per thousand.

Example: Although we are currently collecting the theoretical ingredients needed for statistical tests to be described in detail later on, we briefly pause, taking a look at a very simple example of a statistical test.

Suppose that a carefully maintained base line is known to have a length of 151.723 m. This value has been verified so many times that we regard it as free of any error. Suppose that a newly delivered distance meter gives a reading of 151.745. The manufacturers specified a standard deviation (root mean square error) of 5 mm, if the distance is in the range of 150 m. We make the following hypothesis: (1) The distance meter is free of any systematic error. (2) No severe blunder occurred during the measurement. (3) The r.m.s. error of 5 mm specified by the company is correct. (4) The observations are normally distributed.

We test the hypothesis as follows. If it is true, our observation is normally distributed with mean 151.723 and standard deviation 5 mm. The observed value 151.745 is outside the 3σ- boundaries (which are $151.723 \pm 0.015 = 151.708$ and 151.738 respectively). Hence we <u>reject</u> the hypothesis.

Statistical tests to be described later are modelled after this simple case. However the distribution functions involved are more complicated, and we have to learn more about them. Nevertheless, some preliminary questions are posed here:

*) Why do we choose the critical area of rejection as $|X-\mu| > 3\sigma$, and not otherwise, for example as $X-\mu > 3\sigma$, or even as $|X-\mu| >$ some constant?

*) A not rejected hypothesis is <u>not</u> always considered as accepted without reservations. Additional information may lead to rejection at a later time.

*) The probability of rejecting a true hypothesis is in our case given by 0.0027. A more difficult question is: How large is the probability to accept a wrong hypothesis. Obviously the probability depends on <u>how</u> wrong the hypothesis is.

1.2. The multidimensional Gauss distribution (normal distribution).

Let the random variable X be n- dimensional having a density function:

$$f(x) = f\left(x_1, \ldots, x_n\right) =$$

$$= \frac{1}{(2\pi)^{n/2}} |A|^{1/2} \exp\left[-\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} \left(x_i-\mu_i\right) \left(x_j-\mu_j\right)\right]$$

$$= \frac{1}{(2\pi)^{n/2}} |A|^{1/2} \exp\left[-\frac{1}{2} (x-\mu)^T A (x-\mu)\right]$$

Thereby the matrix $A = (a_{ij})$ is symmetric and positive definite. The symbol $|A|$ denotes the determinant of A, which is positive. The vector

$$\mu = \left(\mu_1, \ldots, \mu_n\right)^T$$

can be verified to be the vector of mean values

$$E(X) = \mu$$

The inverse

$$\Sigma = A^{-1}$$

can be verified to be the covariance matrix of X

$$\Sigma(X) = \Sigma = A^{-1}$$

Remark: The case n=1 reduces to the one- dimensional Gauss distribution described in the previous section. Just identify $\mu=\mu_1$, $\Sigma={a_{11}}^{-1}=\sigma^2$.

Theorems on the multidimensional Gauss distribution: (without proofs)

(1) Marginal distribution. Each component X_i of X can be viewed as a one-dimensional random variable (cf. section B.2.5.). As such, X_i has a one-dimensional Gauss distribution with mean $E(X_i) = \mu_i$ and variance $\sigma^2(X_i) = \sigma_{ii}$, the i-th diagonal element of Σ.

More generally: Partition X as

$$X = \begin{bmatrix} X_{(1)} \\ X_{(2)} \end{bmatrix}$$

where $X_{(1)}$ and $X_{(2)}$ are vectors of size n_1, n_2; $n_1+n_2=n$.

Partition μ, accordingly

$$\mu = \begin{bmatrix} \mu_{(1)} \\ \mu_{(2)} \end{bmatrix}, \qquad \Sigma = \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}$$

Then X_i has an n_i- dimensional Gauss distribution with mean μ_i and covariance matrix Σ_{ii}; i=1,2

$$f\left(x_{(i)}\right) = \frac{1}{(2\pi)^{n_i/2}} \exp\left(-\frac{1}{2}\left(x_{(i)} - \mu_{(i)}\right)^T A_{ii}\left(x_{(i)} - \mu_{(i)}\right)\right),$$

$$A_{ii} = \Sigma_{ii}^{-1}, \quad i=1,2$$

(2) Linear functions of normally distributed random variables. Let

$$Y = BX + b$$

be a linear, inhomogeneous function of X, which is assumed normally distributed with $E(X)=\mu$, $\Sigma(X)=\Sigma$. Then Y is also normally distributed with

$$E(Y) = B\mu + b, \; \Sigma(Y) = B\Sigma(X)B^T = B\Sigma B^T$$

Note that E(Y), $\Sigma(Y)$ follow from the propagation laws for expectations and covariances given in section B.3.7.

(3) Meaning of zero correlation in case of normally distributed random variables. Assume that $\Sigma=\Sigma(X)$ is of the form

$$\Sigma(X) = \begin{bmatrix} \sigma_{11} & & & \\ & \sigma_{22} & & 0 \\ & 0 & \cdot & \\ & & & \cdot \\ & & & & \sigma_{nn} \end{bmatrix} = \begin{bmatrix} \sigma_1^2 & & & \\ & \sigma_2^2 & & 0 \\ & 0 & \cdot & \\ & & & \cdot \\ & & & & \sigma_n^2 \end{bmatrix}$$

Then the components of X are mutually uncorrelated. As a consequence

$$A = \Sigma^{-1} = \begin{bmatrix} a_{11} & & & \\ & a_{22} & & 0 \\ & 0 & \cdot & \\ & & & \cdot \\ & & & & a_{nn} \end{bmatrix} = \begin{bmatrix} 1/\sigma_1^2 & & & \\ & 1/\sigma_2^2 & & 0 \\ & 0 & \cdot & \\ & & & \cdot \\ & & & & 1/\sigma_n^2 \end{bmatrix}$$

The probabilty density presents itself as

$$f(x) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left(- \frac{(x_i-\mu_i)^2}{2\sigma_i^2}\right)$$

This is true because

$$|A| = \left[\sigma_1^2 \ \sigma_2^2 \ \ldots \ \sigma_n^2\right]^{-1}$$

and

$$\exp\left(- \frac{1}{2} (x-\mu)^T A^{-1} (x-\mu)\right) = \exp\left(- \frac{1}{2} \sum_{i=1}^{n} a_{ii} \ (x_i-\mu_i)^2\right)$$

$$= \prod_{i=1}^{n} \exp\left(- \frac{1}{2} \frac{(x_i-\mu_i)^2}{\sigma_i^2}\right)$$

It is seen that f(x) decomposes as

$$f(x) = f_{(1)}(x_1) \ f_{(2)}(x_2) \ \ldots \ f_{(n)}(x_n)$$

where $f_{(i)}(x_i)$ is the marginal density of the component X_i. In view of section B.2.6. we recognize that the components X_i of X are mutually stochastically <u>independent</u>.

Thus: In case of normally distributed random variables zero correlation means stochastic independence.

This generalizes to the following situation. Split X, μ again as

$$X = \begin{bmatrix} X_{(1)} \\ X_{(2)} \end{bmatrix}, \qquad \mu = \begin{bmatrix} \mu_{(1)} \\ \mu_{(2)} \end{bmatrix}$$

Assume that Σ is of the form

$$\Sigma = \begin{bmatrix} \Sigma_{11} & 0 \\ 0 & \Sigma_{22} \end{bmatrix}$$

Then the random variables $X_{(1)}$, $X_{(2)}$, whose marginal densities $f_{(1)}\left(x_{(1)}\right)$, $f_{(2)}\left(x_{(2)}\right)$ have been specified under (1), are independent. It holds that

$$f(x) = f_{(1)}\left(x_{(1)}\right)\, f_{(2)}\left(x_{(2)}\right)$$

<u>Remark:</u> An important special case arises if $\mu_i=0$, $\sigma_{ii}=\sigma^2$, $\sigma_{ij}=0$, $i \neq j$. The components X_i of X are then identically and <u>independently distributed</u>. We have $\mu=0$, $\Sigma=I\sigma^2$. Any component has the Gauss distribution with mean zero and variance σ^2. If observations of the same kind are taken under identical circumstances, then the observation errors are frequently assumed to be distributed in this way.

<u>1.3. The chi- squared distribution (χ^2- distribution).</u>

Let $X_1,\ldots,X_n$ be mutually independent and normally distributed random variables, having mean $E\left(X_i\right)=0$ and $\sigma^2\left(X_i\right)=1$. Thus any X_i has the normalized Gauss distribution, and the random vector $X=(X_1,\ldots,X_n)^T$ has mean and covariance matrix given by

$$E(X) = 0 \,, \qquad \Sigma(X) = I$$

We consider the function of X

$$\chi^2_n = \Phi(X) = X_1{}^2 + X_2{}^2 + \ldots + X_n{}^2$$

This is a <u>nonlinear</u> function which may also be written as

$$\chi^2_n = X^T X$$

The random variable χ^2_n has a distribution which is called chi- squared (χ^2) distribution with n degrees of freedom. An analytical expression may be specified, but is not needed here. It holds that

$$E(\chi^2_n) = n$$
$$\sigma^2(\chi^2_n) = 2n$$

The proof of $E(\chi^2_n)=n$ is easy: Since any X_i has the normalized Gauss distribution, we have $E(X_i)=0$ and

$$E(X_i{}^2) = E\{(X_i-E(X_i))^2\} = \sigma^2(X_i) = 1$$

Hence the random variable X_i^2 has expectation $E(X_i^2)=1$. The random variable χ^2_n is the sum of n such random variables. Hence its expectation must be n- times as large (Remember: the expectation operator is linear; cf. section B.3.7.).

The distribution functions $F_{\chi^2_n}(x)$ are tabulated for moderately large values of n (n<200, for example). For large values of n, $F_{\chi^2_n}(x)$ approximates a Gauss distribution with mean n and variance 2n.

Note that $\chi^2_n \geq 0$. Hence $F_{\chi^2_n}(x)=0$ for x<0.

1.4. Student's distribution (t- distribution).

Let X_i, i=1,...,n again be random variables being mutually independent, and obeying the normalized Gauss distribution. Let Y be another random variable having the normalized Gauss distribution, and let Y be independent of any X_i. Thus the partitioned random vector

$$\begin{bmatrix} X \\ Y \end{bmatrix} = \begin{bmatrix} X_1 \\ \cdot \\ \cdot \\ X_n \\ Y \end{bmatrix}$$

has expectation and covariance given by

$$E\begin{bmatrix} X \\ Y \end{bmatrix} = 0, \qquad \Sigma\begin{bmatrix} X \\ Y \end{bmatrix} = I$$

We consider the function

$$t_n = \frac{Y}{\sqrt{(X_1^2+X_2^2+...+X_n^2)/n}}$$

The distribution of this nonlinear function t_n of X, Y is called Student's distribution, or t- distribution with n degrees of freedom.

<u>Remark:</u> Note that the denominator can be written as

$$\sqrt{(X_1^2+...+X_n^2)/n} = \sqrt{\chi^2{}_n/n}$$

where $\chi^2{}_n$ is a random variable having the χ^2- distribution introduced in the previous subsection.

Student's distribution has a density whose analytical representation is not given here. It is symmetric with respect to the origin t_n=0. The distribution function is tabulated for moderately large n (again, n<200 is reasonable). For large n it approximates the normalized Gauss distribution.

1.5. Fisher's distribution (F- distribution).

Let $X_1,...,X_m$, $Y_1,...,Y_n$ be mutually independent random variables having the normalized Gauss distribution. The quantity

$$F_{m,n} = \frac{(X_1^2+...+X_m^2)/m}{(Y_1^2+...+Y_n^2)/n}$$

is a random variable whose distribution is called Fisher's F- distribution with m and n degrees of freedom.

Remark: Note that $F_{m,n}$ is represented as

$$F_{m,n} = \frac{\chi^2_m/m}{\chi^2_n/n}$$

i.e. as the quotient of two normalized and independent χ^2- distributed random variables having m and n degrees of freedom.

The F- distribution is tabulated for moderately large n and m (n,m<200, say). If n becomes very large, the denominator can be considered to be a constant with value 1. The numerator is then χ^2_m divided by m. If m becomes very large, the argument can be applied to $1/F_{m,n}=F_{n,m}$.

2. Canonical transformation.

2.1. Preliminaries.

We consider an adjustment problem in the Gauss- Markoff form

$$E(\ell) = Ax, \qquad \Sigma(\ell) = Q\sigma^2$$

Alternatively, we also consider the conventional form

$$\ell+v = Ax, \qquad \Sigma(\ell) = Q\sigma^2$$

which shows the corrections explicitely. We assume ℓ of dimension n, x of dimension m, such that A is an n*m matrix, whereby m<n and rank(A)=m.

We subject the problem to a series of transformations such that from the final appearance not only the solution can be read off immediately, but also various statistical quantities needed in tests to be described later. Our transformation will be a more sophisticated version of the transformation described in section A.8.5. It will only serve the purpose of mathematical proofs and theoretical insight. In practical application such transformations are never carried out explicitely.

Our transformations will not only involve the quantities ℓ, v, Ax, Q, σ^2 showing up in the above problem formulation. We also consider a set of p linear functionals

$$\phi = \Phi x$$

defined on the subspace L_A which is spanned by the columns of A. The rows of the p*m matrix Φ represent linear functions of the unknown parameters x.

Statistical tests to be described later will be concerned with hypotheses like

$$\Phi x = c$$

where c is a vector of p constants.

2.2. Making the functionals a part of the parameters.

We augment the p*m matrix Φ by an (m-p)*m matrix Ψ such that

$$C = \begin{bmatrix} \Phi \\ \Psi \end{bmatrix}$$

becomes an m*m regular matrix. We introduce new parameters

$$y = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

by

$$y = Cx, \qquad \text{or} \quad y_1 = \Phi x, \quad y_2 = \Psi x$$

The inverse transformation is

$$x = C^{-1}y$$

and our adjustment problem transforms as

$$\ell+v = AC^{-1}y$$

or

$$\ell+v = \bar{A}y, \quad \bar{A} = AC^{-1}$$

or

$$\ell+v = \bar{A}_1 y_1 + \bar{A}_2 y_2$$

The first set of parameters refers now directly to the p functionals: $y_1=\Phi x$.

<u>2.3. Orthogonal decomposition of the space L_A.</u>

As usual, we view the realizations of ℓ, as well as $\lambda=E(\ell)$, the columns of A, $\bar{A}$, as members of an inner product space L. The inner product is represented by

$$P = Q^{-1}$$

Note that A and $\bar{A}$ span the subspace L_A (the columns of $\bar{A}$ are linear combinations of those of A). In an analogous way as described in section A.9.3. on partial reduction, we decompose the space $L_A=L_{\bar{A}}$ into ortho- complementary subspaces $L_{\bar{A}_1}$ and $L_{\bar{A}_2}$. The only change with respect to section A.9.3. is an additional overbar over the A_i's, and an interchange of the subscripts 1 and 2. As we know from the cited section, the orthogonal decomposition goes along with a parameter transformation

$$y_1 = y_1$$
$$z_2 = y_2 - \left(\bar{A}_2{}^T P \bar{A}_2\right)^{-1} \bar{A}_2{}^T P \bar{A}_1 \; y_1$$

The result is the transformed problem

$$\ell + v = \bar{\bar{A}}_1 y_1 + \bar{A}_2 z_2 ,$$

with

$$\bar{\bar{A}}_1 = \bar{A}_1 - \bar{A}_2 \left(\bar{A}_2{}^T P \bar{A}_2\right)^{-1} \bar{A}_2{}^T P \bar{A}_1 = \left(I - P_{\bar{A}_2}\right) \bar{A}_1$$

and

$$\bar{\bar{A}}_1{}^T P \bar{A}_2 = 0$$

2.4. Orthogonal decomposition of L into L_A and L_B.

Such a transformation has been used in several earlier sections. It is accomplished by

$$\ell = \left(\bar{\bar{A}}_1 , \bar{A}_2 , B\right) \ell'$$

or

$$\ell' = \begin{bmatrix} \ell_1' \\ \ell_2' \\ \ell_3' \end{bmatrix} = \begin{bmatrix} \left(\bar{\bar{A}}_1{}^T P \bar{\bar{A}}_1\right)^{-1} \bar{\bar{A}}_1{}^T P \\ \left(\bar{A}_2{}^T P \bar{A}_2\right)^{-1} \bar{A}_2{}^T P \\ \left(B^T P B\right)^{-1} B^T P \end{bmatrix} \ell$$

Shortly

$$\ell' = S\ell$$

The matrix B fulfills $A^TPB=0$, and also $\bar{\bar{A}}_1{}^TPB=0$, $\bar{A}_2{}^TPB=0$. Our adjustment problem transforms into

$$\begin{aligned} \ell_1'+v_1' &= y_1 \\ \ell_2'+v_2' &= z_2 \,, \\ \ell_3'+v_3' &= 0 \end{aligned} \qquad \Sigma(\ell') = \begin{bmatrix} \left(\bar{\bar{A}}_1{}^TP\bar{\bar{A}}_1\right)^{-1} & 0 & 0 \\ 0 & \left(\bar{A}_2{}^TP\bar{A}_2\right)^{-1} & 0 \\ 0 & 0 & \left(B^TPB\right)^{-1} \end{bmatrix} \sigma^2$$

Already at this step we see that the best estimates and corrections are

$$\begin{aligned} y_1 &= \ell_1', & v_1' &= 0 \\ z_2 &= \ell_2', & v_2' &= 0 \\ & & v_3' &= -\ell_3' \end{aligned}$$

<u>Remark:</u> Recall the geometric interpretation of this transformation. A new basis is chosen in L. The new basis is the union of bases in $L_{\bar{\bar{A}}_1}$, $L_{\bar{A}_2}$, L_B. These 3 subspaces are orthogonal. The inner product in L was represented by P with respect to the old bases. With respect to the new bases it is represented by

$$P' = \begin{bmatrix} \bar{\bar{A}}_1{}^TP\bar{\bar{A}}_1 & 0 & 0 \\ 0 & \bar{A}_2{}^TP\bar{A}_2 & 0 \\ 0 & 0 & B^TPB \end{bmatrix}$$

The reproducing kernel is represented by

$$Q' = (P')^{-1}$$

Consequently

$$\Sigma(\ell') = Q'\sigma^2$$

Note also the validity of the error propagation law:

$$\ell' = S\ell, \quad \Sigma(\ell') = S\Sigma(\ell)S^T, \quad \Sigma(\ell) = Q\sigma^2$$

2.5. Orthonormalizing the bases of the subspaces.

Let V be a vector space; let $e_1, \ldots, e_n$ be a basis, and let the positive definite matrix G represent the inner product. As outlined in section A.4.7., a set of orthonormal vectors $e_1', \ldots, e_n'$ may be derived. If these vectors are chosen as new basis vectors, the coordinates of vectors transform as

$$x = R^{-1}x'$$

(The earlier notation used in section A.3.2., paragraph (6) was $x_{OLD} = Ax_{NEW}$.). The inner product with respect to the new basis is represented by the identity matrix

$$G' = \left(R^{-1}\right)^T G R^{-1} = I$$

We see that G is represented as

$$G = R^T R$$

<u>Remark:</u> There is a very old, very practical and well- known procedure to compute the matrix G. It is the method by Cholesky. R is the Cholesky- factor of G. R is an upper triangular matrix (cf. section D.3.).

The inner products in our 3 subspaces $L_{\bar{\bar{A}}_1}$, $L_{\bar{A}_2}$, L_B are represented by

$$G_1 = \bar{\bar{A}}_1{}^T P \bar{\bar{A}}_1$$
$$G_2 = \bar{A}_2{}^T P \bar{A}_2$$
$$G_3 = B^T P B$$

We factorize these matrices as

$$G_1 = R_1{}^T R_1$$
$$G_2 = R_2{}^T R_2$$
$$G_3 = R_3{}^T R_3$$

We accordingly transform the observations by

$$\ell_1'' = R_1 \ell_1'$$
$$\ell_2'' = R_2 \ell_2'$$
$$\ell_3'' = R_3 \ell_3'$$

Shortly

$$\ell'' = S'\ell'$$

Our adjustment problem transforms into

$$\begin{aligned} \ell_1''+v_1'' &= R_1 y_1 \\ \ell_2''+v_2'' &= \qquad R_2 z_2 \\ \ell_3''+v_3'' &= \qquad\qquad 0 \end{aligned} \quad , \qquad \Sigma\begin{vmatrix} \ell_1'' \\ \ell_2'' \\ \ell_3'' \end{vmatrix} = \begin{vmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & I \end{vmatrix} \sigma^2$$

<u>Remark:</u> The described transformations imply an alternative form of the final stage given by

$$\begin{aligned} E\left(\ell_1''\right) &= R_1 y_1 \\ E\left(\ell_2''\right) &= \qquad R_2 z_2 \\ E\left(\ell_3''\right) &= \qquad\qquad 0 \end{aligned}$$

with $\Sigma(\ell'')$ as given above.

The solution is

$$\begin{aligned} y_1 &= R_1^{-1}\ell_1'', & v_1'' &= 0 \\ z_2 &= R_2^{-1}\ell_2'', & v_2'' &= 0 \\ & & v_3'' &= -\ell_3'' \end{aligned}$$

The covariances of the various quantities are

$$\Sigma(y_1) = (R_1^{-1})(R_1^{-1})^T \sigma^2 = (R_1^T R_1)^{-1} \sigma^2 = G_1^{-1} \sigma^2$$
$$\Sigma(z_2) = (R_2^T R_2)^{-1} \sigma^2$$
$$\Sigma(v_3'') = I \sigma^2$$

Because a change of basis in L amounts to an isometric transformation (cf. section A.8.4.2.), we have

$$\|v\|^2 = v^T P v = \|v_3''\|^2 = \|\ell_3''\|^2 = (\ell_3'')^T \ell_3''$$

Because $y_1 = \Phi x$, we see that y_1 is the BLUE for the functionals $\phi = \Phi x$. On the other hand, the BLUE for Φx can also be obtained conventionally by adjusting for the x's directly

$$x = (A^T P A)^{-1} A^T P \ell$$

with

$$\Sigma(x) = (A^T P A)^{-1} \sigma^2$$

and

$$y_1 = \Phi x$$

with

$$\Sigma(y_1) = \Sigma(\Phi x) = \Phi (A^T P A)^{-1} \Phi^T \sigma^2$$

Thus we see

$$G_1^{-1} = \left(R_1^{T} R_1\right)^{-1} = \Phi\left(A^{T} P A\right)^{-1} \Phi^{T}$$

This formula will help us to utilize the insight gained through canonical transformation without actually performing this transformations in practical calculations.

3. Distribution of various quantities resulting from a least squares adjustment.

3.1. The joint distribution of BLUE'S and of the residuals.

We now make the decisive assumption that the observations ℓ are normally distributed. Thus the vector ℓ is assumed to have an n- dimensional Gauss distribution with mean $E(\ell)=\lambda=Ax$ and covariance matrix $\Sigma(\ell)=Q\sigma^2$.

We see that the mean is specified in terms of m unknown parameters x. The covariance may also have an unknown parameter, namely σ^2. However, σ^2 may also be assumed to be known.

The best estimates of functionals $\Phi=\phi x$ are given by

$$\tilde{\Phi} = \phi\tilde{x} = \phi\left(A^TPA\right)^{-1}A^TP\ell$$

The residuals are given by

$$v = -\left(I - A\left(A^TPA\right)^{-1}A^TP\right)\ \ell$$

$\tilde{\Phi}$ as well as v are linear functions of the observation ℓ. Hence they are also normally distributed (cf. section 1.2., paragraph (2)). In order to specify their multidimensional normal distribution, it suffices to specify the vector of expectations and the covariance matrix. Because the $\tilde{\Phi}$ are BLUE's we have

$$E(\tilde{\Phi}) = \Phi = \phi x$$

This may also be verified directly. On the other hand

$$E(v) = 0$$

as one recognizes by applying the E- operator to the above expressions for v and by recalling $E(\ell)=Ax$.

A straightforward application of the error propagation law (for covariances) yields:

$$\Sigma\begin{bmatrix}\tilde{\Phi}\\ v\end{bmatrix} = \begin{bmatrix}\Phi\left(A^TPA\right)^{-1}\Phi^T & 0\\ 0 & Q-A\left(A^TPA\right)^{-1}A^T\end{bmatrix}\sigma^2$$

It is seen that the BLUE's $\tilde{\Phi}=\Phi\tilde{x}$ and the residuals v are uncorrelated and, since we deal with normal distributions, stochastically <u>independent.</u>

<u>3.2. Distribution of the "weighted sum of residuals".</u>

The quantity

$$v^TPv$$

is the quantity which is minimized during least squares adjustment. Its distribution will now be specified.

<u>Theorem:</u> The quantity

$$\frac{1}{\sigma^2} v^T P v = \frac{1}{\sigma^2} \sum_{i=1}^{n} \sum_{j=1}^{n} p_{ij} v_i v_j$$

has a χ^2_{n-m} distribution, i.e. a χ^2- distribution with n-m degrees of freedom.

Remark: n is the number of observations, m is the number of unknown parameters; hence

n-m

is the number of redundant observations.

Proof: We refer to section 2.5. There the equation

$$(v^T P v) = (\ell_3'')^T \ell_3''$$

was listed. The vector ℓ_3'' has n-m components. The expectation of ℓ_3'' is zero (this is stated in remark within section 2.5.).

The covariance of ℓ_3'' is $I\sigma^2$. Hence the covariance of $(1/\sigma)\ell_3''$ is I. It follows that

$$\frac{1}{\sigma^2} (\ell_3'')^T \ell_3'' = \frac{1}{\sigma^2} v^T P v$$

is a sum of squares of n-m independent random variables having a normalized Gauss distribution. Thus the sum has the χ^2_{n-m} distribution. Confer the definition of χ^2 in section 1.3.

3.3. Expressions in $\Phi\tilde{x}$ and v having the χ^2- or the F- distribution.

The following theorem is fundamental for statistical tests of linear hypotheses.

Theorem: Let $\Phi\tilde{x}$ be the BLUE for Φx, where Φ is a p*m matrix. Denote

$$c = \Phi x$$

Then

$$\chi^2_p = \frac{1}{\sigma^2} (\Phi\tilde{x}-c)^T \left(\Phi\left(A^TPA\right)^{-1}\Phi^T\right)^{-1} (\Phi\tilde{x}-c)$$

has a χ^2- distribution with p degrees of freedom. Furthermore

$$F_{p,n-m} = \frac{(\Phi\tilde{x}-c)^T \left(\Phi\left(A^TPA\right)^{-1}\Phi^T\right)^{-1} (\Phi\tilde{x}-c)/p}{\left(v^TPv\right)/(n-m)}$$

has an F- distribution with p and n-m degrees of freedom.

Remark: The quantity $c=\Phi x$ is unknown because the x are unknown. Hence χ^2_p and $F_{p,n-m}$ involve the unknown quantity c. However the distribution of χ^2_p and $F_{p,n-m}$ is known. In later sections hypothetical values for c will be specified, and these hypotheses will be tested using the specified expressions and their distributions.

Proof: In section 2.5. we have seen that

$$\ell_1'' = R_1\tilde{y}_1 = R_1\Phi\tilde{x}$$
$$E(\ell_1'') = R_1 y_1 = R_1\Phi x = R_1 c$$
$$\Sigma(\ell_1'') = I\sigma^2$$

Hence

$$\frac{1}{\sigma^2}\left[\ell_1''-E(\ell_1'')\right]^T\left[\ell_1''-E(\ell_1'')\right]$$

is a sum of squares of p independent random variables (the components of $(1/\sigma)\left[\ell_1''-E(\ell_1'')\right]$), having the normalized Gauss distribution. By the definition of the χ^2- distribution, the above expression is a χ^2_p. Substituting for ℓ_1'' and $E(\ell_1'')$ we obtain

$$\chi^2_p = \frac{1}{\sigma^2}\left(R_1\Phi\tilde{x}-R_1c\right)^T\left(R_1\Phi\tilde{x}-R_1c\right) =$$

$$= \frac{1}{\sigma^2}(\Phi\tilde{x}-c)^T R_1^T R_1 (\Phi\tilde{x}-c)$$

In section 2.5. it was noted that

$$R_1^T R_1 = G_1 = \left(\Phi\left(A^TPA\right)^{-1}\Phi^T\right)^{-1}$$

This proves the assertion on χ^2_p.

The assertion on $F_{p,n-m}$ is proved similarly by noting that $(1/\sigma)\left[\ell_1''-E(\ell_1'')\right]$ and $(1/\sigma)\ell_3''$ represent p + n-m random variables having the normalized Gauss distribution.

Hence

$$F_{p,n-m} = \frac{[\ell_1''-E(\ell_1'')]^T\,[\ell_1''-E(\ell_1'')]/p}{(\ell_3''^T\ell_3'')/(n-m)}$$

has the F- distribution with p and n-m degrees of freedom. Recalling that $(\ell_3'')^T\ell_3''=v^TPv$ makes the proof complete.

<u>Theorem:</u> (Alternative representation of the quantities χ^2_p and $F_{p,n-m}$ specified in the previous theorem.) Let v be the residuals of the adjustment problem

$$\ell+v = Ax, \qquad \Sigma(\ell) = Q\sigma^2$$

Let v_c be the residuals of this adjustment problem augmented by p additional constraints:

$$\begin{aligned} \ell+v_c &= Ax, \qquad \Sigma(\ell) = Q\sigma^2 \\ c &= \Phi x \end{aligned}$$

Here c is viewed as a vector of constants (the constraints may e.g. be used to reduce the number of parameters). Then

$$(\Phi\tilde{x}-c)^T\,\left(\Phi\left(A^TPA\right)^{-1}\Phi^T\right)^{-1}\,(\Phi\tilde{x}-c) = v_c{}^TPv_c - v^TPv$$

Hence

$$\chi^2_p = \frac{1}{\sigma^2}\left(v_c{}^TPv_c-v^TPv\right)$$

and

$$F_{p,n-m} = \frac{\left(v_c{}^T P v_c - v^T P v\right)/p}{\left(v^T P v\right)/(n-m)}$$

are the same quantities as those listed in the preceding theorem.

<u>Remark:</u> The newly specified expressions for $\chi^2{}_p$ and $F_{p,n-m}$ are frequently easier to calculate by means of available computer programs for least squares adjustment.

<u>Proof:</u> Just note from the canonical transformation that

$$v^T P v = \left(\ell_3''\right)^T \ell_3''$$

Next we must show that

$$v_c{}^T P v_c = \left(\ell_1''-R_1 c\right)^T \left(\ell_1''-R_1 c\right) + \left(\ell_3''\right)^T \ell_3''$$

This expression is verified by noting that the canonical transformation of the modified problem is

$$\begin{aligned} \ell_1''+v_1'' &= R_1 c \\ \ell_2''+v_2'' &= \quad R_2 z_2 \ , \qquad \Sigma(\ell'') = I\sigma^2 \\ \ell_3''+v_3'' &= \qquad 0 \end{aligned}$$

The obvious solution of this problem is

$$v_1'' = -\left(\ell_1''-R_1c\right)$$

$$z_2 = R_2^{-1}\ell_2'', \quad v_2'' = 0$$

$$v_3'' = -\ell_3''$$

Due to isometry we have $v_c^T P v_c = \left(v''\right)^T v''$. Thus

$$v_c^T P v_c = \left(\ell_1''-R_1c\right)^T \left(\ell_1''-R_1c\right) + \left(\ell_3''\right)^T \ell_3''$$

and the proof is completed by plugging it into the proof at the preceding theorem.

3.4. Expressions in $\tilde{x}$ and v having the t- distribution.

A random variable $F_{1,n-m}$ having the F- distribution with 1 and n-m degrees of freedom can be seen as the square of a random variable t_{n-m} having the t- distribution with n-m degrees of freedom. Hence the following theorem is very closely related to the second assertion of the first theorem of the preceding section. In the following theorem we assume p=1, and we write Φx as $\phi^T x$.

Theorem: Let $\Phi=\phi^T x$ be a linear function of the unknowns and let $\tilde{\Phi}=\phi^T\tilde{x}$ be its BLUE.Put

$$\phi^T x = c$$

Then

$$t_{n-m} = \frac{\left(\phi^T\tilde{x}-c\right)}{\sqrt{\phi^T\left(A^TPA\right)^{-1}\phi\ \left(v^TPv\right)/(n-m)}}$$

has the t- distribution with n-m degrees of freedom.

Proof: Replace in section 2 the quantity Φx by $\Phi^T x$ everywhere. Then ℓ_1'' has only one component. It follows that

$$t_{n-m} = \frac{\ell_1'' - E(\ell_1'')}{\sqrt{(\ell_3'')^T \ell_3'' / (n-m)}}$$

is a t_{n-m}. Resubstituting for ℓ_1'' and ℓ_3'' gives the stated expression.

4. Confidence regions.

4.1. Confidence intervals for one- dimensional Gauss variables.

Suppose that X has the one- dimensional Gauss distribution with unknown expectation $\mu=E(X)$ and known standard deviation $\sigma=\sigma(X)$. As described in section 1.1., a transformation is made whose effect is a replacement of X by a random variable

$$\Xi = \frac{X-\mu}{\sigma}$$

having the normalized Gauss distribution. One specifies a certain probabiltiy α which is usually chosen close to 1. Values of $\alpha=0.9$, $\alpha=0.95$, $\alpha=0.99$ are common choices. The probability α is called confidence level. Using a table of the normalized Gauss distribution, one determines k_α such that

$$p\left\{-k_\alpha \leqslant \Xi \leqslant k_\alpha\right\} = \alpha$$

This is equivalent to

$$p\left\{-k_\alpha \leqslant \frac{X-\mu}{\sigma} \leqslant k_\alpha\right\} = \alpha$$

or

$$p\left\{X-k_\alpha\sigma \leqslant \mu \leqslant X+k_\alpha\sigma\right\} = \alpha$$

It is seen that an interval has been specified whose boundaries are random variables. The interval covers the unknown expectation μ with a prescribed probability α. The interval carries the name confidence interval.

4.2. Application to the Gauss- Markoff model with known unit weight error.

Consider the familiar Gauss- Markoff model

$$E(\ell) = Ax, \quad \Sigma(\ell) = Q\sigma^2, \quad P = Q^{-1}$$

Assume that σ^2 is known. Hence $\Sigma(\ell)$ is completely known. Consider a functional Φ and its BLUE $\tilde{\Phi}$

$$\Phi = \phi^T x, \qquad \tilde{\Phi} = \phi^T \tilde{x}$$

The distribution of $\tilde{\Phi}$ is a Gauss distribution with unknown expectation

$$E(\tilde{\Phi}) = \Phi = \phi^T x$$

and with standard deviation

$$\sigma(\tilde{\Phi}) = \sqrt{\phi^T \left(A^T P A\right)^{-1} \phi}\; \sigma$$

The previous subsection describes how to specify a confidence interval for Φ: Choose a confidence level α, ask a table or a computer for k_α, and specify the interval

$$\tilde{\Phi} - k_\alpha \sqrt{\phi^T \left(A^T P A\right)^{-1} \phi}\; \sigma \leqslant \Phi \leqslant \tilde{\Phi} + k_\alpha \sqrt{\phi^T \left(A^T P A\right)^{-1} \phi}\; \sigma$$

or

$$\tilde{\Phi} - k_\alpha \sigma(\tilde{\Phi}) \leq \Phi \leq \tilde{\Phi} + k_\alpha \sigma(\tilde{\Phi})$$

It covers the unknown value Φ with a probability α.

A special choice ϕ^T is the j-th row of the unit matrix:
In this case

$$\Phi = \phi^T x = x_j$$

the j-th component of the vector of unknown parameters. It holds that

$$\sigma^2(\tilde{x}_j) = \phi^T (A^T P A)^{-1} \phi \; \sigma^2 = q_{x_j x_j} \; \sigma^2$$

where $q_{x_j x_j}$ is the j-th diagonal element of the inverse normal equation matrix

$$Q_{xx} = (A^T P A)^{-1}$$

The confidence interval is

$$\tilde{x}_j - k_\alpha \sqrt{q_{x_j x_j}} \; \sigma \leq x_j \leq \tilde{x}_j + k_\alpha \sqrt{q_{x_j x_j}} \; \sigma$$

or

$$\tilde{x}_j - k_\alpha \sigma(\tilde{x}_j) \leq x_j \leq \tilde{x}_j + k_\alpha \sigma(\tilde{x}_j)$$

Another special choice of ϕ^T is:

$$\phi^T = \left(a_{i1}, \ldots, a_{im}\right)$$

i.e. the i-th row of the design matrix A. In this way, one can derive a confidence interval for the i-th component λ_i of the vector

$$\lambda = E(\ell)$$

Remark: Nobody can prevent a person from specifying confidence intervals for a multitude of functionals $\phi^T x$. For example confidence intervals for all parameters x_i, $i=1,\ldots,m$ and/or for all observables λ_i, $i=1,\ldots,n$ could be computed and displayed. One has to be careful not to interpret these confidence intervals and their associated confidence levels in a wrong way. In order to illustrate possible pitfalls, assume 2 confidence intervals, one for x_1, the first parameter, and one for x_2, the second parameter. We then have

$$p\left\{\tilde{x}_1 - k_\alpha \sigma\left(\tilde{x}_1\right) \le x_1 \le \tilde{x}_1 + k_\alpha \sigma\left(\tilde{x}_1\right)\right\} = \alpha$$

$$p\left\{\tilde{x}_2 - k_\alpha \sigma\left(\tilde{x}_2\right) \le x_2 \le \tilde{x}_2 + k_\alpha \sigma\left(\tilde{x}_2\right)\right\} = \alpha$$

The meaning of these equations is the following one. Suppose that the process of taking observations ℓ and computing estimates $\tilde{x}$ is repeated N times, where N is large. Then approximately in $N\alpha$ cases the first confidence interval covers x_1, and also in $N\alpha$ cases the second interval covers x_2. It is however not clear in how many cases both intervals cover appropriate values simultaneously. Thus the probability of the joint event

$$\{\tilde{x}_1 - k_\alpha\sigma(\tilde{x}_1) \le x_1 \le \tilde{x}_1 + k_\alpha\sigma(\tilde{x}_1),\ \tilde{x}_2 - k_\alpha\sigma(\tilde{x}_2) \le x_2 \le \tilde{x}_2 + k_\alpha\sigma(\tilde{x}_2)\}$$

is unknown. This probability would be α^2 if $\tilde{x}_1$ and $\tilde{x}_2$ were independent. It would be α, if they were completely dependent (i.e. if $\tilde{x}_2$ were a function of $\tilde{x}_1$). Generally $\tilde{x}_1$ and $\tilde{x}_2$ are correlated. Hence the probability for the joint event is somewhere between the specified limits. We shall see later how ellipsoidal confidence regions can be specified which cover both x_1 and x_2 with a pre-specified probability α.

4.3. Studentization.

Consider now the Gauss- Markoff model

$$E(\ell) = Ax, \qquad \Sigma(\ell) = Q\sigma^2$$

where σ is now assumed as <u>unknown</u>. If $\Phi=\phi^T x$ is a functional, then its BLUE is

$$\tilde{\Phi} = \phi^T\tilde{x}$$

as before. The variance is

$$\sigma^2(\tilde{\Phi}) = \phi^T\left(A^T PA\right)^{-1}\phi\ \sigma^2$$

It is unknown, because σ^2 is unknown. We are used to estimate σ^2 by

$$\frac{v^T P v}{n-m} = \tilde{\sigma}^2$$

The estimate $\tilde{\sigma}^2$ for σ is unbiased. From section 3.2. we know that $\left(1/\sigma^2\right)v^T Pv$ is a χ^2_{n-m}. Hence $E\left(v^T Pv\right)=(n-m)\sigma^2$. Thus

$$E\left(\tilde{\sigma}^2\right) = \sigma^2$$

We denote by $\tilde{\sigma}$ the square root of $\tilde{\sigma}^2$ (we cannot claim that $E(\tilde{\sigma})=\sigma$, but $\tilde{\sigma}$ appears to be a reasonable estimate for σ).

We also denote

$$\tilde{\sigma}(\tilde{\Phi}) = \sqrt{\phi^T\left(A^T PA\right)^{-1}\phi}\;\tilde{\sigma}$$

Thus $\tilde{\sigma}(\tilde{\Phi})$ is an estimate for $\sigma(\tilde{\Phi})$. The crucial point is now that

$$t_{n-m} = \frac{\tilde{\Phi}-\Phi}{\tilde{\sigma}(\tilde{\Phi})}$$

has Student's t- distribution with n-m degrees of freedom. The proof is given by the theorem of section 3.4. Just mind that $\tilde{\Phi} = \phi^T\tilde{x}$, that $\Phi=\phi^T x$ has been denoted by c, and that the denominator of the expression in the theorem of section 3.4. is nothing but $\tilde{\sigma}(\tilde{\Phi})$.

We are now able to specify a confidence interval for ϕ. After prescribing α, one uses a table of the t- distribution to find k_α such that

$$p\left\{-k_\alpha \leq t_{n-m} \leq k_\alpha\right\} = \alpha$$

Thus

$$p\left\{-k_\alpha \leq \frac{\tilde{\phi}-\phi}{\tilde{\sigma}(\tilde{\phi})} \leq k_\alpha\right\} = \alpha$$

or

$$p\left\{\tilde{\phi} - k_\alpha\tilde{\sigma}(\tilde{\phi}) \leq \phi \leq \tilde{\phi} + k_\alpha\tilde{\sigma}(\tilde{\phi})\right\} = \alpha$$

Thus a ramdom interval has been specified which covers the unknown value $\phi=\phi^T x$ with a prespecified probability.

4.4. Confidence regions for σ^2.

The quantity

$$\tilde{\sigma}^2 = \frac{v^T P v}{n-m}$$

was seen to be an unbiased estimator for σ^2.

Further more, in section 3.2. it was seen that

$$\chi^2_{n-m} = (n-m)\,\frac{\tilde{\sigma}^2}{\sigma^2} = \frac{v^T P v}{\sigma^2}$$

has the χ^2- distribution with n-m degrees of freedom. Confidence regions for σ^2 may be constructed as follows.

(1) Two- sided confidence interval. After specifying the confidence level α, choose q_α and r_α such that

$$p\{q_\alpha > \chi^2_{n-m}\} = p\{\chi^2_{n-m} > r_\alpha\} = \frac{1-\alpha}{2}$$

Then

$$p\{q_\alpha \leq \chi^2_{n-m} \leq r_\alpha\} = \alpha$$

or

$$p\{q_\alpha \leq (n-m)\frac{\tilde{\sigma}^2}{\sigma^2} \leq r_\alpha\} = \alpha$$

or

$$p\{(n-m)\frac{\tilde{\sigma}^2}{r_\alpha} \leq \sigma^2 \leq (n-m)\frac{\tilde{\sigma}^2}{q_\alpha}\} = \alpha$$

(2) One- sided confidence interval of finite size. Choose q_α such that

$$p\{q_\alpha \leq \chi^2_{n-m}\} = \alpha$$

Then

$$p\{\sigma^2 \leq (n-m)\frac{\tilde{\sigma}^2}{q_\alpha}\} = \alpha$$

(3) One- sided confidence interval of infinite size. Choose r_α such that

$$p\{\chi^2_{n-m} \leq r_\alpha\} = \alpha$$

Then

$$p\{\sigma^2 \geq (n-m)\frac{\tilde{\sigma}^2}{r_\alpha}\} = \alpha$$

The choice of a confidence interval of type (1), (2), (3) depends on the situation. If one is suspicious against σ^2 which are either too small or too large, then (1) is chosen. If one is suspicious against σ^2 which are too large, then (2) is chosen. Similarly for (3).

4.5. Ellipsoidal confidence regions for sets of linear estimates.

We consider a set of p linear functions

$$\phi = \Phi x$$

together with their BLUE's

$$\tilde{\phi} = \Phi \tilde{x}$$

The matrix Φ is of size p*m. From section 3.3. we know that

$$\chi^2_p = \frac{1}{\sigma^2} (\Phi\tilde{x}-\Phi x)^T \left(\Phi\left(A^T PA\right)^{-1}\Phi^T\right)^{-1} (\Phi\tilde{x}-\Phi x)$$

$$= (\tilde{\phi}-\phi)^T \; \Sigma(\tilde{\phi})^{-1} \; (\tilde{\phi}-\phi)$$

has the χ^2- distribution with p degrees of freedom.

We also know that

$$F_{p,n-m} = \frac{(\Phi\tilde{x}-\Phi x)^T \left(\Phi\left(A^T PA\right)^{-1}\Phi^T\right)^{-1} (\Phi\tilde{x}-\Phi x)/p}{\left(v^T Pv\right)/(n-m)}$$

$$= (\tilde{\phi}-\phi)^T \; \tilde{\Sigma}(\tilde{\phi})^{-1} \; (\tilde{\phi}-\phi)/p$$

has an F- distribution with p and n-m degrees of freedom. In these formulas we denote as usual

$$\Sigma(\tilde{\Phi}) = \Phi\left(A^T PA\right)^{-1}\Phi^T\ \sigma^2 \ \ldots \text{ covariance of } \tilde{\Phi} = \Phi\tilde{x}$$

$$\tilde{\sigma}^2 \quad = \left(v^T Pv\right)/(n-m) \quad \ldots \text{ estimate for } \sigma^2$$

$$\tilde{\Sigma}(\tilde{\Phi}) = \Phi\left(A^T PA\right)^{-1}\Phi^T\ \tilde{\sigma}^2 \ \ldots \text{ estimate for } \Sigma(\tilde{\Phi})$$

The above formulae put us into the position to specify ellipsoidal confidence regions when σ is either known or unknown.

(1) σ^2 known. Choose a confidence level α, find k_α such that

$$p\left\{\chi^2_{\ p} \leq k_\alpha\right\} = \alpha$$

Then

$$p\left\{(\tilde{\Phi}-\Phi)^T\ \Sigma(\tilde{\Phi})^{-1}\ (\tilde{\Phi}-\Phi) \leq k_\alpha\right\} = \alpha$$

The matrix $\Sigma(\tilde{\Phi})^{-1}$ is known and positive definite.

If M is any p*p positive definite matrix then all points (position vectors) x fulfilling

$$\left(x_0-x\right)^T\ M\ \left(x_0-x\right) = c_0$$

are situated on a p- dimensional ellipsoid. The ellipsoid has its center at x_0. The directions of the axes are the directions of the eigenvectors of M. The lengths of the axes are given by the square roots of c_0 divided by the eigenvalues of M. The points x fulfilling

$$\left(x_0-x\right)^T M \left(x_0-x\right) \leq c_0$$

are situated in the interior and at the boundary of the above ellipsoid.

If we interprete $\tilde{\Phi}$ and Φ as position vectors of points, we see that all points Φ fulfilling

$$(\tilde{\Phi}-\Phi)^T \Sigma(\tilde{\Phi})^{-1} (\tilde{\Phi}-\Phi) \leq k_\alpha$$

are situated in the interior and at the boundary of a p- dimensional ellipsoid centered at $\tilde{\Phi}$. Thus we have specified an ellipsoidal region which covers the unknown p- dimensional point Φ with a prespecified probability α.

(2) σ^2 unknown. Choose α and k_α such that

$$p\left\{F_{p,n-m} \leq k_\alpha\right\} = \alpha$$

i.e.

$$p\left\{(\tilde{\Phi}-\Phi)^T \tilde{\Sigma}(\tilde{\Phi})^{-1} (\tilde{\Phi}-\Phi)/p \leq k_\alpha\right\} = \alpha$$

Hence an ellipsoidal region has been specified covering the unknown point Φ in p- dimensional space with prescribed probability.

5. Tests of linear hypotheses.

5.1. Linear hypotheses.

We again start from the familiar Gauss- Markoff model for n observations and m unknowns

$$E(\ell) = Ax, \quad \Sigma(\ell) = Q\sigma^2, \quad P = Q^{-1}$$

The unit weight error σ may be known or unknown. A linear hypotheses is a system of p linear equations of the form

$$\Phi x = c$$

The vector c is comprised of p pre- specified constants. One could say that a linear hypothesis assumes that p linear functionals Φx on L_A (the space of adjusted observations) have certain pre- specified values c. This assumption is usually called the "null hypothesis". The "alternative hypothesis" would be that $\Phi x \neq c$.

The usual procedure to test the null hypothesis is the following one. The BLUE $\tilde{x}$ for x is an m- dimensional random variable. It has the multidimensional Gauss distribution with (unknown) mean x and covariance matrix $\Sigma(\tilde{x})$. $\Sigma(\tilde{x})$ may be known or unknown. In the latter case $\tilde{\Sigma}(\tilde{x})$ is an estimate for $\Sigma(\tilde{x})$. $\left(\tilde{\Sigma}(\tilde{x})=\left(A^TPA\right)^{-1}\tilde{\sigma}^2,\ \tilde{\sigma}^2=v^TPv/(n-m)\right)$. The m- dimensional space R^m of realizations of $\tilde{x}$ is divided into two regions, a region of acceptance and a region of rejection. If the outcome of $\tilde{x}$ is in the region of acceptance, the null hypothesis is accepted (with some reservations). If $\tilde{x}$ is in the region of rejection, the null hypothesis is rejected (definitely).

As regions of acceptance the confidence intervals of chapter 4 may be used with the roles of Φ and $\tilde{\Phi}$ interchanged. The region of acceptance is thus an ellipsoid centered at $\Phi=c$. The region of rejection is the complementary region. It is seen that a certain probability α is associated with a test. $1-\alpha$ is the probability of rejecting a true null hypothesis. In section 4 on confidence intervals, α was called "level of confidence". Now we call $1-\alpha$ the "level of significance".

Rejecting a true null hypothesis is called "error of the first kind". The probability of accepting a false hypothesis, i.e. the probability of an "error of the second kind", is more difficult to specify. It depends on "how wrong" the null hypothesis is, i.e. it depends on $\Phi x-c$. If $\Phi x-c$ is small, then the probability of an error of the second kind is near α, and is therefore quite large. This is the reason wy acceptance of the null hypothesis is done with some reservation. A subsequent, larger sample could lead to rejection of an earlier accepted hypothesis.

5.2. Tests of variances.

If σ^2 is unknown, an estimate $\tilde{\sigma}^2$ is available as

$$\tilde{\sigma}^2 = \frac{v^T P v}{n-m}$$

One can adopt the null hypothesis

$$\sigma^2 = \sigma_0{}^2$$

where $\sigma_0{}^2$ is a pre- specified value. The null hypothesis can be tested by means of the χ^2- distribution with n-m degrees of freedom. One specifies a level of significance $1-\alpha$ which is small. Recall that α was called confidence level in section 4. As explained in section 4.4., one finds q_α and r_α such that

$$p\left[q_\alpha \leq (n-m)\,\frac{\tilde{\sigma}^2}{\sigma_0{}^2} \leq r_\alpha\right] = \alpha$$

The interval

$$q_\alpha \leq (n-m)\,\frac{\tilde{\sigma}^2}{\sigma_0{}^2} \leq r_\alpha \quad \text{or} \quad \frac{q_\alpha}{n-m}\,\sigma_0{}^2 \leq \tilde{\sigma}^2 \leq \frac{r_\alpha}{n-m}\,\sigma_0{}^2$$

is the region of acceptance. The complementary region is the region of rejection.

Remark: If one is suspicious that σ_0 might have been specified as too small, one is better advised to use a one sided region of acceptance. One finds r_α such that

$$p\left[(n-m)\,\frac{\tilde{\sigma}^2}{\sigma_0{}^2} \leq r_\alpha\right] = \alpha$$

and uses the region of acceptance

$$\tilde{\sigma}^2 \le \frac{r_\alpha}{n-m}\,\sigma_0^{\ 2}$$

5.3. A simple example.

A base line used for comparison measurements has a known length of 151.723 m. A newly delivered distance meter gives values ℓ_i, i=1,...,20 listed in table 5.1. The company specifies a standard deviation (root mean square error) of σ=5mm.

i	ℓ_i	v_i*10^4	i	ℓ_i	v_i*10^4
1	151.745	- 105	11	151.752	- 175
2	.743	- 85	12	.730	+ 45
3	.728	+ 65	13	.724	+ 105
4	.728	+ 65	14	.711	+ 235
5	.744	- 95	15	.745	- 105
6	.724	+ 105	16	.738	- 35
7	.739	- 45	17	.730	+ 45
8	.721	+ 135	18	.733	+ 15
9	.744	- 95	19	.738	- 35
10	.731	+ 35	20	.742	- 75

Table 5.1

Reading of a distance meter for a base line with known length of 151.723 m's.

We first check the hypothesis σ=5mm. We perform an adjustment whose Gauss-Markoff model is

$$E(\ell_i) = x \quad i = 1,\ldots,n \quad , \qquad \Sigma(\ell_i) = I\sigma^2$$

This is the model for direct observations of equal accuracy, the most elementary model of least squares adjustment.

The BLUE $\tilde{x}$ for x is the arithmetic mean

$$x = \frac{1}{20} \sum_{i=1}^{20} \ell_i = 151.734_5 \text{ m}$$

We calculate corrections (residuals) v_i which are also shown in table 5.1. One computes

$$\tilde{\sigma}^2 = \frac{1}{19} v^T v = \frac{1975}{19} \text{ mm}^2 = 103.9_5 \text{ mm}^2$$

$$\sigma = 10.2 \text{ mm}$$

We are suspicious that σ_0 has been specified to small. Hence we perform a one-sided test as explained in the remark at the end of the previous subsection. Under the null hypothesis $\sigma=\sigma_0$=5mm the quantity

$$(n-m) \frac{\tilde{\sigma}^2}{\sigma_0^2} = 19 \frac{\tilde{\sigma}^2}{\sigma_0^2} = \frac{v^T v}{\sigma_0^2} = \chi^2{}_{19}$$

has a χ^2- distribution with n-m (=19) degrees of freedom. Taking 1-α=0.05, i.e. α=0.95, and using a table for the χ^2 distribution, we find

$$p\{\chi^2{}_{19} \leqslant 30.1\} = 0.95$$

or

$$p\left\{19\,\frac{\tilde{\sigma}^2}{\sigma_0^{\;2}} \leq 30.1\right\} = 0.95$$

or

$$p\left\{\tilde{\sigma}^2 \geq \frac{30.1}{19}\,\sigma_0^{\;2}\right\} = 0.05$$

The region of rejection is

$$\tilde{\sigma}^2 \geq \frac{30.1}{19}\,\sigma_0^{\;2}$$

or

$$\tilde{\sigma} \geq 1.26\sigma_0 = 6.29 \text{ mm}$$

Our value σ=10.2mm is in the region of rejection. Thus the hypothesis $\sigma=\sigma_0$ is rejected. We use $\tilde{\sigma}$=10.2mm instead of σ_0=5mm in further tests.

Remark: Note that there is no reason to put all the blame on the company. It may have been that the instrument was not used according to the specifications.

Our next null hypothesis concerns the measured length of the base line. We postulate that

$$E(\tilde{x}) = 151.723 \text{ m} = c$$

Thus the null- hypothesis assumes that the baseline has been measured without any systematic error. We need information on the variance of $\tilde{x}$. Because σ_0=5mm has been rejected, we do not calculate

$$\sigma^2(\tilde{x}) = \frac{1}{20}\,\sigma_0{}^2 = 1.25 \text{ mm}^2$$

but we rather estimate

$$\tilde{\sigma}^2(\tilde{x}) = \frac{1}{20}\,\tilde{\sigma}^2 = \frac{(10.2)^2}{20} \text{ mm}^2 = 5.20 \text{ mm}^2$$

or

$$\tilde{\sigma}(\tilde{x}) = 2.3 \text{ mm}$$

Under the null hypothesis the quantity

$$\frac{\tilde{x}-c}{\tilde{\sigma}(\tilde{x})}$$

whose observed value is

$$\frac{151.734_5 - 151.723}{0.0023} = 5.0$$

has a t- distribution with 19 degrees of freedom. Confer sections 3.4. and 4.3. Using a table for the t- distribution we find

$$p\{-2.09 \leq t_{19} \leq 2.09\} = 0.95$$

It is seen that the null hypothesis is rejected.

The region of acceptance can also be displayed as:

$$151.723 - 2.09*0.0023 \leq \tilde{x} \leq 151.723 + 2.09*0.0023$$

or

$$151.718_1 \text{ m} \leq \tilde{x} \leq 151.727_8 \text{ m}$$

The value $\tilde{x}=151.734_5$m is outside this range. We conclude that either the instrument is wrong, or that the base line has changed its length, or that the measurement was biased for some reason.

5.4. A sophisticated example.

It shall be tested whether a dam is subsiding as time goes on. After finishing the construction of the dam the leveling network shown in fig.5.1 was measured. It will be called the time 1- network.

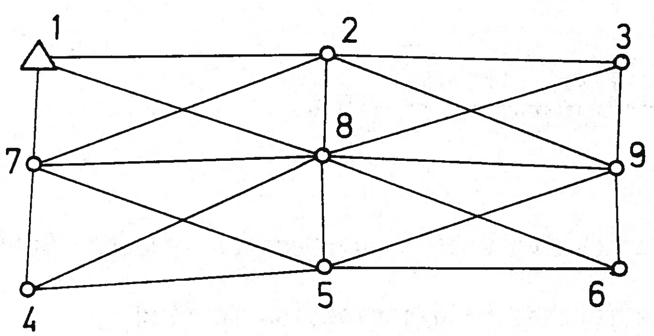


Fig.5.1 Time 1- network

The points 7,8,9 are situated on the dam. The other points 1,...,6 are located on firm ground. The height of point 1 is assumed to be known.

After the lapse of some time (one year maybe), new levelings were carried out. The same instrument and rods were used, the same observer as well. Also otherwise it was attempted to measure under the same conditions as they were given during the first measurement. This justifies the assumption that the unit weight error was the same for both time periods.

Not all height differences were releveled at the second time. The network for the second measurement (i.e. the time 2- network) looked as shown in fig.5.2.

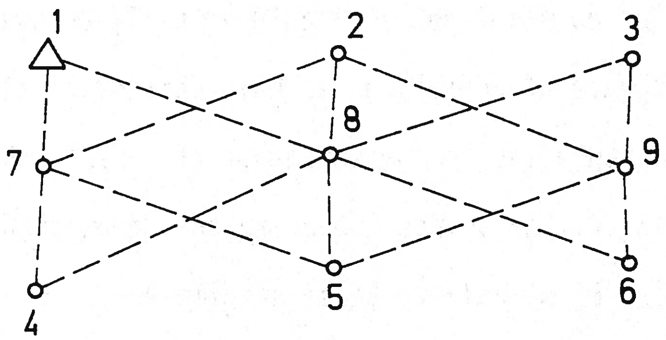


Fig.5.2 Time 2- network

The null hypothesis postulates that the heights of points 7,8,9 did not change. Rejection of the null hypothesis means that at least one height has changed.

The procedure for testing the null hypothesis goes on as follows. Both networks are combined, whereby the points 7,8,9 are duplicated by considering points 7',8',9' in addition. The unprimed points refer to time 1, the primed points refer to time 2. The combined network looks as shown in fig.5.3.

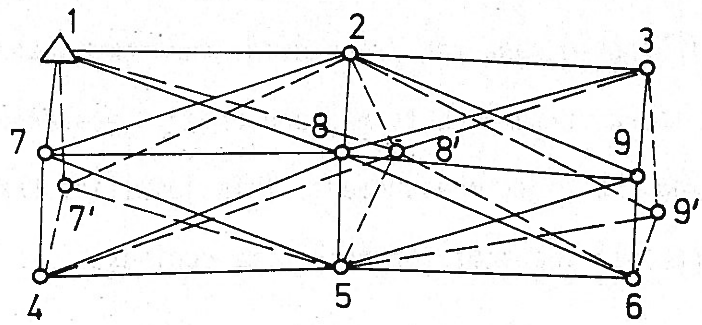


Fig.5.3 Combined network

Note that the points 7 and 7' should actually be drawn on top of each other. However for ease of comparison we have shifted 7' slightly away from 7. The solid lines represent the measurements at time 1, the dashed lines represent those at time 2. The points 7,8,9 are only connected to measurements at time 1, the points 7',8',9' only to those at time 2.

The combined network is now adjusted in agreement with the Gauss- Markoff model

$$E(\ell) = Ax, \qquad \Sigma(\ell) = I\sigma^2$$

We have n=34 and m=11, n-m=23. The vector of parameters x comprises the height of the points 2,3,4,5,6,7,8,9,7',8',9'

$$x = \left(H_2,\ H_3,\ H_4,\ H_5,\ H_6,\ H_7,\ H_8,\ H_9,\ H_{7'},\ H_{8'},\ H_{9'}\right)^T$$

From the vector of 34 residuals we calculate

$$v^T v = \sum_{i=1}^{34} v_i^2$$

We compute the estimate of the unit weight error

$$\tilde{\sigma} = \sqrt{\frac{v^T v}{34-11}} = \sqrt{\frac{v^T v}{23}}$$

The covariance of the adjusted heights is estimated as

$$\tilde{\Sigma}(\tilde{x}) = \left(A^T A\right)^{-1} \tilde{\sigma}^2$$

The null hypothesis is the following linear hypothesis

$$H_7 = H_{7'}$$
$$H_8 = H_{8'}$$
$$H_9 = H_{9'}$$

or

$$H_7 - H_{7'} = 0$$
$$H_8 - H_{8'} = 0$$
$$H_9 - H_{9'} = 0$$

or

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 \end{bmatrix} x = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

This is denoted

$$\Phi x = c = 0, \qquad \text{i.e. } c = 0$$

The best estimates for Φx are

$$\Phi\tilde{x}$$

whereby $\tilde{x}$ comprises the adjusted heights

$$\tilde{x} = \left(\tilde{H}_2, \tilde{H}_3, \tilde{H}_4, \tilde{H}_5, \tilde{H}_6, \tilde{H}_7, \tilde{H}_8, \tilde{H}_9, \tilde{H}_{7'}, \tilde{H}_{8'}, \tilde{H}_{9'}\right)^T$$

Under the null hypothesis the quantity

$$F_{3,23} = (\Phi\tilde{x})^T \tilde{\Sigma}(\Phi\tilde{x})^{-1} (\Phi\tilde{x})/3$$

with

$$\tilde{\Sigma}(\Phi\tilde{x}) = \Phi\left(A^T A\right)^{-1}\Phi^T \tilde{\sigma}^2$$

has the F- distribution with 3 and 23 degrees of freedom. Specifying a significance level of $1-\alpha=0.05$, and using a table for the F- distribution, one finds

$$p\left\{F_{3,23} \leq 3.03\right\} = 0.95$$

The region of acceptance is therefore given by

$$(\Phi\tilde{x})^T \tilde{\Sigma}(\Phi\tilde{x})^{-1} (\Phi\tilde{x}) \leq 3 * 3.03$$

Remark: The above outlined testing procedure requires the calculation of $\Phi\left(A^T A\right)^{-1}\Phi^T$, which may not be easy if conventional software for least squares adjustment is used. The second theorem of section 3.3. offers another possibility to calculate $F_{3,23}$. From the above adjustment of the combined network one just notes v^Tv. The combined network is then adjusted a second time, whereby the pairs of points (7,7'), (8,8'), (9,9') are identified. This is equivalent to an adjustment of

$$E(\ell) = Ax$$

$$\Phi x = 0$$

with Φ as given above. The equations $\Phi x = 0$ are used to eliminate $H_{7'}$, $H_{8'}$, $H_{9'}$, so to speak.

Thus, during the second adjustment, one has only 8 parameters instead of 11. These parameters are

$$\left(H_2,\ H_3,\ H_4,\ H_5,\ H_6,\ H_7,\ H_8,\ H_9\right)^T$$

From the residuals v_c of the second adjustment one calculates $v_c{}^T v_c$.

According to the second theorem of section 3.3., the quantity

$$F_{3,23} = \frac{(v_c^T v_c - v^T v)/3}{(v^T v)/23}$$

is the same as that one used in the earlier procedure.

<u>Problem</u>: Our null hypothesis was: "The heights of the points 7,8,9 did not change". The alternative hypothesis was therefore "At least one height changed". A change of height is either a decrease or an increase. One may wish to exclude the possibility of increasing heights on a dam which is expected to subside. Hence the null hypothesis could be formulated differently as follows: "The heights of points 7,8,9 did not decrease". Can you imagine a test procedure for this modified null hypothesis?

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