Appendix A
Rank of Matrices

A matrix $\boldsymbol{A}$ is said to have rank r if there is at least one non-zero sub-determinant of order $(r \times r)$ while all sub-determinants of higher order are zero. The notation is $\text{rank}(\boldsymbol{A}) = r$.

The system or design matrix $\boldsymbol{A}$, referred to in the method of least squares, Sect. 9.2, has m rows and r columns, $m > r$. Given $\boldsymbol{A}$ has rank r, its r columns are linearly independent.

It appears advantageous to consider the columns of a matrix as vectors. Obviously, $\boldsymbol{A}$ has r m-dimensional column vectors. Let us denote the latter by $\boldsymbol{a}_k$; $k = 1, \ldots, r$. If the $\boldsymbol{a}_k$ are independent, they span an r-dimensional subspace $R(\boldsymbol{A}) = V_m^r(\Re)$ of the m-dimensional space $V_m(\Re)$ wherein $\Re$ denotes the set of real numbers.

1. $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$, Sect. 9.2

Let $\text{rank}(\boldsymbol{A}) = r$ and the $\boldsymbol{a}_k$; $k = 1, \ldots, r$ be a basis of an r-dimensional subspace $R(\boldsymbol{A}) = V_m^r(\Re)$ of $V_m(\Re)$. Due to the independence of the $\boldsymbol{a}_k$, it is not possible to find a vector

$$\boldsymbol{\beta} = \begin{pmatrix}\beta_1 & \beta_2 & \cdots & \beta_r\end{pmatrix}^{\mathrm{T}} \neq \mathbf{0}$$

so that

$$\boldsymbol{A}\boldsymbol{\beta} = \beta_1\boldsymbol{a}_1 + \beta_2\boldsymbol{a}_2 + \cdots + \beta_r\boldsymbol{a}_r = \mathbf{0}\,.$$

The vector

$$\boldsymbol{c} = \beta_1\boldsymbol{a}_1 + \beta_2\boldsymbol{a}_2 + \cdots + \beta_r\boldsymbol{a}_r$$

is in the column space of the matrix $\boldsymbol{A}$. Consequently, the vector $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{c}$ must be different from the zero vector, as $\boldsymbol{c}$ cannot be orthogonal to all vectors $\boldsymbol{a}_k$; $k = 1, \ldots, r$. But if for any vector $\boldsymbol{\beta} \neq \mathbf{0}$

$$\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\,\boldsymbol{\beta} \neq 0\,,$$

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the columns of $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$ must be independent; thus rank$(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}) = r$. Moreover, as $(\boldsymbol{A}\boldsymbol{\beta})^{\mathrm{T}}\boldsymbol{A}\boldsymbol{\beta}$ equals the squared length of the vector $\boldsymbol{A}\boldsymbol{\beta}$, which is nonzero if $\boldsymbol{\beta}$ is nonzero, we have

$$\boldsymbol{\beta}^{\mathrm{T}}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)\boldsymbol{\beta} > 0 .$$

Hence, the real symmetric matrix $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$ is positive definite.

2. $\boldsymbol{P} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}$*, Sect. 9.2*

The rank of an idempotent matrix, $\boldsymbol{P}^2 = \boldsymbol{P}$, is equal to its trace [60]. Given the product of two matrices, say $\boldsymbol{R}$ and $\boldsymbol{S}$, is defined in either way, $\boldsymbol{R}\boldsymbol{S}$ and $\boldsymbol{S}\boldsymbol{R}$, we have trace$(\boldsymbol{R}\boldsymbol{S}) =$ trace$(\boldsymbol{S}\boldsymbol{R})$, i.e.

$$\begin{aligned}\operatorname{rank}\left(\boldsymbol{P}\right) &= \operatorname{trace}\left(\boldsymbol{P}\right)\\ &= \operatorname{trace}\left[\boldsymbol{A}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}\right] = \operatorname{trace}\left[\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\right] = r .\end{aligned}$$

3. $\boldsymbol{C} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{H}^{\mathrm{T}}$*, Sect. 9.3*

Putting $\boldsymbol{B} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}$, whereat rank$(\boldsymbol{B}) = r$, we have

$$\operatorname{rank}\left(\boldsymbol{C}\right) \le \min\left[\operatorname{rank}\left(\boldsymbol{B}\right), \operatorname{rank}\left(\boldsymbol{H}^{\mathrm{T}}\right)\right] = q .$$

Hence, rank$(\boldsymbol{C}) = q$.

4. $\boldsymbol{B}^{\mathrm{T}}\boldsymbol{s}\,\boldsymbol{B}$*, Sect. 12.2*

As we confine ourselves to positive definite empirical variance–covariance matrices $\boldsymbol{s}$, we may resort to a decomposition $\boldsymbol{s} = \boldsymbol{c}^{\mathrm{T}}\boldsymbol{c}$ at what $\boldsymbol{c}$ denotes a non-singular $(m \times m)$ matrix [59]. Due to $\boldsymbol{B}^{\mathrm{T}}\boldsymbol{s}\,\boldsymbol{B} = (\boldsymbol{c}\,\boldsymbol{B})^{\mathrm{T}}(\boldsymbol{c}\,\boldsymbol{B})$, the symmetric matrix $\boldsymbol{B}^{\mathrm{T}}\boldsymbol{s}\,\boldsymbol{B}$ is positive definite, given rank $(\boldsymbol{c}\,\boldsymbol{B}) = r$. Hence, we are indeed in a position to dispose of ellipsoids as introduced by Hotelling.

Appendix B
Variance–Covariance Matrices

Let us turn to m random variables X_i, $\mu_i = E\{X_i\}$; $i = 1, \ldots, m$ and m nonzero real numbers ξ_i; $i = 1, \ldots, m$ and consider the expectation

$$E\left\{\left[\sum_{i=1}^{m} \xi_i (X_i - \mu_i)\right]^2\right\} \geq 0\,. \tag{B.1}$$

For a moment, we reduce the summation to $m = 2$,

$$\left[\sum_{i=1}^{m} \xi_i (X_i - \mu_i)\right]^2$$

$$= \xi_1^2 (X_1 - \mu_1)^2 + 2\,\xi_1 \xi_2 (X_1 - \mu_1)(X_2 - \mu_2) + \xi_2^2 (X_2 - \mu_2)^2$$

so that

$$E\left\{\left[\sum_{i=1}^{m} \xi_i (X_i - \mu_i)\right]^2\right\} = \xi_1^2 \sigma_1^2 + 2\,\xi_1 \xi_2 \sigma_{12} + \xi_2^2 \sigma_2^2 \geq 0\,. \tag{B.2}$$

This, obviously, is a quadratic form. Letting the ξ_1, ξ_2 define a column vector,

$$\boldsymbol{\xi} = (\xi_1 \quad \xi_2)^{\mathrm{T}}\,,$$

and the $\sigma_{11} \equiv \sigma_1^2$, $\sigma_{12} \equiv \sigma_{21}$, $\sigma_{22} \equiv \sigma_2^2$ a theoretical variance–covariance matrix,

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix}\,,$$

being, by its very nature, real and symmetric, (B.2) takes the form

$$\boldsymbol{\xi}^{\mathrm{T}} \boldsymbol{\sigma}\, \boldsymbol{\xi} \geq 0\,. \tag{B.3}$$

If $\boldsymbol{\xi}^{\mathrm{T}} \boldsymbol{\sigma}\, \boldsymbol{\xi} > 0$ for all non-zero vectors $\boldsymbol{\xi}$, the quadratic form is said to be *positive definite*. If, by contrast, there are vectors $\boldsymbol{\xi} \neq \mathbf{0}$ issuing $\boldsymbol{\xi}^{\mathrm{T}} \boldsymbol{\sigma}\, \boldsymbol{\xi} = 0$, the quadratic form is said to be *positive semi-definite*.

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Returning to m variables, we have

$$\boldsymbol{\xi} = (\xi_1 \quad \xi_2 \quad \dots \quad \xi_m)^{\mathrm{T}}$$

and further

$$\sigma_{ij} = E\left\{(X_i - \mu_i)\left(X_j - \mu_j\right)\right\}\,; \quad i, j = 1, \dots, m$$

so that

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \dots & \sigma_{1m} \\ \sigma_{21} & \sigma_{22} & \dots & \sigma_{2m} \\ \dots & \dots & \dots & \dots \\ \sigma_{m1} & \sigma_{m2} & \dots & \sigma_{mm} \end{pmatrix}. \tag{B.4}$$

In view of (B.1), we observe $\boldsymbol{\xi}^{\mathrm{T}}\boldsymbol{\sigma}\,\boldsymbol{\xi} \geq 0$.

At the first, let us consider $\boldsymbol{\xi}^{\mathrm{T}}\boldsymbol{\sigma}\,\boldsymbol{\xi} > 0$. As to that, linear algebra tells us that $\boldsymbol{\sigma}$ is positive definite, implying $\operatorname{rank}(\boldsymbol{\sigma}) = m$. Hence, non-singular theoretical variance–covariance matrices are positive definite. On the other hand, if $\operatorname{rank}(\boldsymbol{\sigma}) < m$, there are vectors $\boldsymbol{\xi} \neq \mathbf{0}$ rendering $\boldsymbol{\xi}^{\mathrm{T}}\boldsymbol{\sigma}\,\boldsymbol{\xi} = \mathbf{0}$ and the quadratic form positive semi-definite.

This treatise confines itself to variance–covariance matrices having full rank. Hence, we may draw on two further results. Let us first recall that a positive definite matrix $\boldsymbol{\sigma}$ requires all eigenvalues to be positive, $\lambda_i > 0\,;\ i = 1, \dots, m$.

– The determinant of $\boldsymbol{\sigma}$ reads

$$|\boldsymbol{\sigma}| = \lambda_1 \cdot \lambda_2 \cdot \dots \cdot \lambda_m > 0\,.$$

– There is a non-singular matrix $\boldsymbol{C}$ such that

$$\boldsymbol{\sigma} = \boldsymbol{C}^T \boldsymbol{C}\,.$$

Finally, let us reconsider $m = 2$ and substitute indices x, y for $1, 2$,

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix}, \quad \sigma_{xx} \equiv \sigma_x^2\,,\ \sigma_{xy} \equiv \sigma_{yx}\,,\ \sigma_{yy} \equiv \sigma_y^2\,.$$

Due to $|\boldsymbol{\sigma}| > 0$, we have $\sigma_{xx}\sigma_{yy} - \sigma_{xy}^2 > 0$ so that we make out the inequality

$$-\sigma_x\sigma_y < \sigma_{xy} < \sigma_x\sigma_y\,.$$

Let us proceed from expectations and theoretical variance–covariance matrices to sums and empirical variance–covariance matrices. To this end, we consider m arithmetic means

$$\bar{x}_i = \frac{1}{n}\sum_{l=1}^{n} x_{il}\,; \quad i = 1, \dots, m$$

each one covering n repeated measurements. We start from

$$\frac{1}{n-1}\sum_{l=1}^{n}\left[\sum_{i=1}^{m}\xi_i\,(x_{il} - \bar{x}_i)\right]^2 \geq 0 \tag{B.5}$$

and let the

$$s_{ij} = \frac{1}{n-1} \sum_{l=1}^{n} (x_{il} - \bar{x}_i)\left(x_{jl} - \bar{x}_j\right)\,; \quad i, j = 1, \ldots, m$$

engender the empirical variance–covariance matrix

$$\boldsymbol{s} = \begin{pmatrix} s_{11} & s_{12} & \ldots & s_{1m} \\ s_{21} & s_{22} & \ldots & s_{2m} \\ \ldots & \ldots & \ldots & \ldots \\ s_{m1} & s_{m2} & \ldots & s_{mm} \end{pmatrix}$$

of the given data sets x_{il}; $i = 1, \ldots, m$; $l = 1, \ldots, n$. Equation (B.5) stipulates

$$\boldsymbol{\xi}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{\xi} \geq 0\,. \tag{B.6}$$

Again, we exclusively confine ourselves to empirical variance–covariance matrices being non-singular, rank$(\boldsymbol{s}) = m$. Hence, given $\boldsymbol{\xi}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{\xi} > 0$, the empirical variance–covariance matrix is positive definite, implying $|\boldsymbol{s}| > 0$. By contrast, in case of rank$(\boldsymbol{s}) < m$, there are vectors $\boldsymbol{\xi} \neq \boldsymbol{0}$ inducing $\boldsymbol{\xi}^{\mathrm{T}} \boldsymbol{s}\, \boldsymbol{\xi} = \boldsymbol{0}$. From there, the quadratic form is said to positive semi-definite.

Finally, let us set $m = 2$ and substitute $s_{xy} \equiv s_{yx}$, s_{xx}, s_{yy} for $s_{12} \equiv s_{21}$, s_{11} and s_{22}, respectively. Then

$$\boldsymbol{s} = \begin{pmatrix} s_{xx} & s_{xy} \\ s_{yx} & s_{yy} \end{pmatrix},$$

provided $|\boldsymbol{s}| > 0$, issues the inequality

$$-s_x s_y < s_{xy} < s_x s_y\,. \tag{B.7}$$

Appendix C
Linear Functions of Normal Variables

Let us investigate the statistical behavior of the sum of two jointly normally distributed variables, say, X and Y, be they dependent or not. Referring to the nomenclature as introduced in Sect. 3.2, we have

$$Z = b_x X + b_y Y \tag{C.1}$$

and, further, $\mu_x = E\{X\}$, $\mu_y = E\{Y\}$, $\sigma_{xx} \equiv \sigma_x^2 = E\{(X - \mu_x)^2\}$, $\sigma_{xy} = E\{(X - \mu_x)(Y - \mu_y)\}$ and $\sigma_{yy} \equiv \sigma_y^2 = E\{(Y - \mu_y)^2\}$.

As usual, the variables X and Y are taken to correspond to measured values, x and y. Putting

$$\boldsymbol{\zeta} = (x \quad y)^{\mathrm{T}}, \quad \boldsymbol{\mu}_{\boldsymbol{\zeta}} = (\mu_x \quad \mu_y)^{\mathrm{T}}, \quad \boldsymbol{b} = (b_x \quad b_y)^{\mathrm{T}}$$

and

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{pmatrix}$$

we arrive at

$$z = \boldsymbol{b}^{\mathrm{T}}\boldsymbol{\zeta}\,, \quad \mu_z = E\{Z\} = \boldsymbol{b}^{\mathrm{T}}\boldsymbol{\mu}_{\boldsymbol{\zeta}}\,, \quad \sigma_z^2 = E\left\{(Z - \mu_z)^2\right\} = \boldsymbol{b}^{\mathrm{T}}\boldsymbol{\sigma}\,\boldsymbol{b}\,.$$

We prove that Z is $N(\mu_z, \sigma_z^2)$ distributed. To this end we refer to method of moment-generating functions, see e.g. [47].

Given a normally distributed variable X, the moment-generating function is defined by

$$M_X(t) = E\left\{\mathrm{e}^{tX}\right\} = \int_{-\infty}^{\infty} \mathrm{e}^{tx}\, p_X(x)\, dx\,, \quad t \in \Re \tag{C.2}$$

whereat according to (3.1)

$$p_X(x) = \frac{1}{\sigma_x\sqrt{2\pi}} \exp\left[-\frac{(x - \mu_x)^2}{2\sigma_x^2}\right].$$

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Strictly speaking, $M_X(t)$ is asked to exist for a certain interval of t including the origin on the real line. Under the condition addressed, this clearly happens to apply.

Adding $\pm\mu_x t$ to the exponent of (C.2), we observe

$$tx - \frac{(x-\mu_x)^2}{2\sigma_x^2} \pm \mu_x t = \mu_x t + \frac{\sigma_x^2 t^2}{2} - \frac{\left[x - (\mu_x + \sigma_x^2 t)\right]^2}{2\sigma_x^2}$$

so that

$$M_X(t) = \exp\left[\mu_x t + \frac{\sigma_x^2 t^2}{2}\right] \int_{-\infty}^{\infty} \frac{1}{\sigma_x\sqrt{2\pi}} \exp\left[-\frac{\left[x - (\mu_x + \sigma_x^2 t\right]^2}{2\sigma_x^2}\right] dx \,.$$

For any admissible t the integral is seen to issue 1. Hence, the moment-generating function of the normally distributed variable X takes the form

$$M_X(t) = \exp\left(\mu_x t + \frac{\sigma_x^2 t^2}{2}\right) . \tag{C.3}$$

Reverting to the moment-generating function of the random variable Z, we have

$$\begin{aligned} M_Z(t) = E\left\{e^{tZ}\right\} &= \int_{-\infty}^{\infty} e^{tz} p_Z(z)\, dz \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \exp\left[t\,(b_x x + b_y y)\right] p\,(x, y)\, dx\, dy \end{aligned} \tag{C.4}$$

wherein

$$p_{XY}(x, y) = \frac{1}{2\pi|\boldsymbol{\sigma}|^{1/2}} \exp\left[-\frac{1}{2}\left(\boldsymbol{\zeta} - \boldsymbol{\mu}_\zeta\right)^{\mathrm{T}} \boldsymbol{\sigma}^{-1}\left(\boldsymbol{\zeta} - \boldsymbol{\mu}_\zeta\right)\right]$$

denotes the joint two-dimensional probability density (3.13). Adding $\pm t\, \boldsymbol{b}^{\mathrm{T}}\boldsymbol{\mu}_\zeta$ to the exponent of (C.4) produces

$$\begin{aligned} & t\,\boldsymbol{b}^{\mathrm{T}}\boldsymbol{\zeta} - \frac{1}{2}\left(\boldsymbol{\zeta} - \boldsymbol{\mu}_\zeta\right)^{\mathrm{T}} \boldsymbol{\sigma}^{-1}\left(\boldsymbol{\zeta} - \boldsymbol{\mu}_\zeta\right) \pm t\,\boldsymbol{b}^{\mathrm{T}}\boldsymbol{\mu}_\zeta \\ &= \boldsymbol{b}^{\mathrm{T}}\boldsymbol{\mu}_\zeta\, t + \frac{\boldsymbol{b}^{\mathrm{T}}\boldsymbol{\sigma}\,\boldsymbol{b}\, t^2}{2} - \frac{1}{2}\left(\boldsymbol{\zeta} - \boldsymbol{\mu}^*\right)^{\mathrm{T}} \boldsymbol{\sigma}^{-1}\left(\boldsymbol{\zeta} - \boldsymbol{\mu}^*\right) \end{aligned}$$

whereat

$$\boldsymbol{\mu}^* = \boldsymbol{\mu}_\zeta + \boldsymbol{\sigma}\,\boldsymbol{b}\,t \,.$$

Taking the exponent carrying the first two terms out of the integral, (C.4) produces

$$\begin{aligned} M_Z(t) = E\left\{e^{tZ}\right\} &= \exp\left(\boldsymbol{b}^{\mathrm{T}}\boldsymbol{\mu}_\zeta t - \frac{\boldsymbol{b}^{\mathrm{T}}\boldsymbol{\sigma}\,\boldsymbol{b}\,t^2}{2}\right) \\ &= \exp\left(\mu_z t - \frac{\sigma_z^2\, t^2}{2}\right) \end{aligned} \tag{C.5}$$

as the remaining integral issues 1.

Obviously, the moment-generating functions (C.3) and (C.5) coincide. As they exist in an interval of t including the origin on the real line, the respective probability densities are equal. Hence, Z is normally distributed with mean μ_z and variance σ_z^2.

Appendix D
Orthogonal Projections

Let $V_m(\Re)$ denote an m-dimensional vector space. Furthermore, let $r < m$ linearly independent vectors

$$\boldsymbol{a}_1 = \begin{pmatrix} a_{11} \\ a_{21} \\ \dots \\ a_{m1} \end{pmatrix}, \quad \boldsymbol{a}_2 = \begin{pmatrix} a_{12} \\ a_{22} \\ \dots \\ a_{m2} \end{pmatrix}, \quad \dots, \quad \boldsymbol{a}_r = \begin{pmatrix} a_{1r} \\ a_{2r} \\ \dots \\ a_{mr} \end{pmatrix}$$

define an r-dimensional subspace $V_m^r(\Re) \subset V_m(\Re)$. Assembling the r vectors within a matrix

$$\boldsymbol{A} = (\boldsymbol{a}_1 \quad \boldsymbol{a}_2 \quad \cdots \quad \boldsymbol{a}_r), \qquad \text{rank}(\boldsymbol{A}) = r,$$

we take that $V_m^r(\Re)$ coincides with the column space $R(\boldsymbol{A})$ of the matrix $\boldsymbol{A}$. The $(m-r)$-dimensional null space $N(\boldsymbol{A}^{\mathrm{T}}) = V_m^{m-r}(\Re)$ of the matrix $\boldsymbol{A}^{\mathrm{T}}$ is orthogonal to $R(\boldsymbol{A})$. The set of linearly independent vectors $\boldsymbol{r}_1, \dots, \boldsymbol{r}_{m-r}$, spanning $N(\boldsymbol{A}^{\mathrm{T}})$, may be drawn from the homogeneous system

$$\boldsymbol{A}^{\mathrm{T}}\boldsymbol{r} = \boldsymbol{0}. \tag{D.1}$$

Every vector of $R(\boldsymbol{A})$ is orthogonal to every vector of $N(\boldsymbol{A}^{\mathrm{T}})$ and vice versa: $V_m(\Re)$ is the direct sum of the subspaces $R(\boldsymbol{A})$ and $N(\boldsymbol{A}^{\mathrm{T}})$,

$$V_m(\Re) = N\left(\boldsymbol{A}^{\mathrm{T}}\right) \oplus R(\boldsymbol{A}).$$

Every vector $\boldsymbol{y}$ of $R(\boldsymbol{A})$ may be uniquely decomposed into a linear combination of the vectors $\boldsymbol{a}_k$; $k = 1, \dots, r$,

$$\boldsymbol{A}\boldsymbol{\beta} = \boldsymbol{y}. \tag{D.2}$$

The r components β_k; $k = 1, \dots, r$ of the vector

$$\boldsymbol{\beta} = (\beta_1 \quad \beta_2 \quad \dots \quad \beta_r)^{\mathrm{T}}$$

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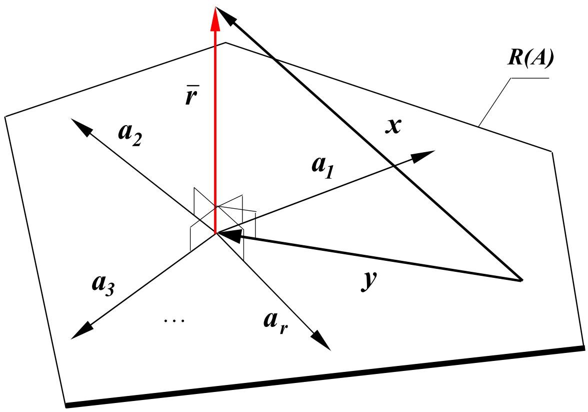

Fig. D.1 The r column vectors $\boldsymbol{a}_1, \boldsymbol{a}_2, \dots, \boldsymbol{a}_r$ span an r-dimensional subspace $R(\boldsymbol{A}) = V_m^r(\Re)$ of the m-dimensional space $V_m(\Re)$. The vector of the residuals, $\bar{\boldsymbol{r}} \in N(\boldsymbol{A}^{\mathrm{T}})$, $N(\boldsymbol{A}^{\mathrm{T}}) \perp R(\boldsymbol{A})$, is orthogonal to the vectors $\boldsymbol{a}_1, \boldsymbol{a}_2 \dots, \boldsymbol{a}_r$

may be conceived as coefficients or "stretch factors" allocating suitable lengths to the vectors $\boldsymbol{a}_k$; $k = 1, \dots, r$ so as to produce

$$\beta_1 \boldsymbol{a}_1 + \beta_2 \boldsymbol{a}_2 + \cdots + \beta_r \boldsymbol{a}_r = \boldsymbol{y} \,.$$

By contrast, let us consider some vector $\boldsymbol{x} \in V_m(\Re)$ referring to an inconsistent, over-determined linear system. Due to the measuring errors, $\boldsymbol{x}$ will not be in $R(\boldsymbol{A})$. Notwithstanding that, we may consider an orthogonal projection of $\boldsymbol{x}$ onto $R(\boldsymbol{A})$, Fig. D.1.—Though seemingly trivial, we like to note: Should, by chance, $\boldsymbol{x}$ lie in $R(\boldsymbol{A})$, a orthogonal projection of $\boldsymbol{x}$ onto $R(\boldsymbol{A})$ would actually effect nothing.

Let $\boldsymbol{P}$ be an operator accomplishing the orthogonal projection of $\boldsymbol{x}$ onto $R(\boldsymbol{A})$ so that

$$\boldsymbol{P}\boldsymbol{x} = \boldsymbol{y} = \boldsymbol{A}\boldsymbol{\beta} \,. \tag{D.3}$$

We shall show that the column vectors $\boldsymbol{a}_k$; $k = 1, \dots, r$ of the matrix $\boldsymbol{A}$ constitute the projection operator $\boldsymbol{P}$. Let $\bar{\boldsymbol{r}} \in N(\boldsymbol{A}^{\mathrm{T}})$ denote the component of $\boldsymbol{x}$ being perpendicular to $R(\boldsymbol{A}) = V_m^r(\Re)$. We have

$$\bar{\boldsymbol{r}} = \boldsymbol{x} - \boldsymbol{y} \,, \quad \boldsymbol{A}^{\mathrm{T}}\bar{\boldsymbol{r}} = \boldsymbol{0} \,. \tag{D.4}$$

Any linear combination of the $m - r$ linearly independent vectors spanning the null space $N(\boldsymbol{A}^{\mathrm{T}}) = V_m^{m-r}(\Re)$ of the matrix $\boldsymbol{A}^{\mathrm{T}}$ is orthogonal to the vectors $\boldsymbol{a}_k$; $k = 1, \dots, r$ spanning the column space $R(\boldsymbol{A}) = V_m^r(\Re)$. By contrast, given $\boldsymbol{P}$, the orthogonal projection $\boldsymbol{y} = \boldsymbol{P}\boldsymbol{x}$ of $\boldsymbol{x}$ onto $R(\boldsymbol{A})$ is fixed so that of all vectors $\boldsymbol{r}$, satisfying $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{r} = \boldsymbol{0}$, $\bar{\boldsymbol{r}} = \boldsymbol{x} - \boldsymbol{P}\boldsymbol{x}$ is singled out.

Assume an orthonormal basis

$$\boldsymbol{\alpha}_1 = \begin{pmatrix} \alpha_{11} \\ \alpha_{21} \\ \dots \\ \alpha_{m1} \end{pmatrix}, \quad \dots, \quad \boldsymbol{\alpha}_m = \begin{pmatrix} \alpha_{1m} \\ \alpha_{2m} \\ \dots \\ \alpha_{mm} \end{pmatrix}$$

of the space $V_m(\Re)$. Let the first r vectors define the column space $R(\boldsymbol{A})$ and let the last $m - r$ span the null space $N(\boldsymbol{A}^{\mathrm{T}})$. Thus, for any vector $\boldsymbol{x} \in V_m(\Re)$ we have

$$x = \underbrace{\gamma_1 \boldsymbol{\alpha}_1 + \cdots + \gamma_r \boldsymbol{\alpha}_r}_{y} \quad + \quad \underbrace{\gamma_{r+1} \boldsymbol{\alpha}_{r+1} + \cdots + \gamma_m \boldsymbol{\alpha}_m}_{\bar{r}} \tag{D.5}$$

$$\boldsymbol{\alpha}_k^{\mathrm{T}} \boldsymbol{x} = \gamma_k \,; \quad k = 1, \ldots, m$$

or

$$\boldsymbol{y} = \sum_{k=1}^{r} \gamma_k \boldsymbol{\alpha}_k \,, \quad \bar{\boldsymbol{r}} = \sum_{k=r+1}^{m} \gamma_k \boldsymbol{\alpha}_k \,.$$

Let the first r vectors $\boldsymbol{\alpha}_k$; $k = 1, \ldots, r$ define the matrix

$$\boldsymbol{T} = \begin{pmatrix} \alpha_{11} & \alpha_{12} & \ldots & \alpha_{1r} \\ \alpha_{21} & \alpha_{22} & \ldots & \alpha_{2r} \\ \ldots & \ldots & \ldots & \ldots \\ \alpha_{m1} & \alpha_{m2} & \ldots & \alpha_{mr} \end{pmatrix}, \quad \boldsymbol{T}^{\mathrm{T}} \boldsymbol{T} = \boldsymbol{I} \tag{D.6}$$

whereat $\boldsymbol{I}$ designates an $(r \times r)$ identity matrix. By contrast, the product $\boldsymbol{T}\boldsymbol{T}^{\mathrm{T}}$ accomplishes the quested orthogonal projection. Indeed, from

$$(\gamma_1 \quad \gamma_2 \quad \cdots \quad \gamma_r)^{\mathrm{T}} = \boldsymbol{T}^{\mathrm{T}} \boldsymbol{x}$$

we find

$$\boldsymbol{y} = \boldsymbol{T} (\gamma_1 \quad \gamma_2 \quad \cdots \quad \gamma_r)^{\mathrm{T}} = \boldsymbol{T}\boldsymbol{T}^{\mathrm{T}} \boldsymbol{x} = \boldsymbol{P}\boldsymbol{x} \,, \quad \boldsymbol{P} = \boldsymbol{T}\boldsymbol{T}^{\mathrm{T}} \,. \tag{D.7}$$

Hence, the projection operator $\boldsymbol{P}$ has been established in terms of an orthonormal basis which, unfortunately, we do not possess.

Meanwhile, we convince ourselves that the projection of any vector $\boldsymbol{y}$ being in $R(\boldsymbol{A})$ gets reproduced. Indeed, from (D.7) we obtain

$$\boldsymbol{P}\boldsymbol{y} = \boldsymbol{T}\boldsymbol{T}^{\mathrm{T}}\boldsymbol{T} (\gamma_1 \quad \gamma_2 \quad \cdots \quad \gamma_r)^{\mathrm{T}} = \boldsymbol{T} (\gamma_1 \quad \gamma_2 \quad \cdots \quad \gamma_r)^{\mathrm{T}} = \boldsymbol{y} \,.$$

In particular, this applies to the column vectors of $\boldsymbol{A}$, hence

$$\boldsymbol{P}\boldsymbol{A} = \boldsymbol{A}. \tag{D.8}$$

Let us revert to the problem of how to express $\boldsymbol{P}$ in terms of the given matrix $\boldsymbol{A}$. To this end, we resort to a non-singular $(r \times r)$ auxiliary matrix

$$\boldsymbol{H} = \boldsymbol{T}^{\mathbf{T}} \boldsymbol{A} \,.$$

Multiplying from the left by $\boldsymbol{T}$ produces $\boldsymbol{T}\boldsymbol{H} = \boldsymbol{T}\boldsymbol{T}^{\mathrm{T}}\boldsymbol{A} = \boldsymbol{P}\boldsymbol{A} = \boldsymbol{A}$, and, further

$$\boldsymbol{T} = \boldsymbol{A}\boldsymbol{H}^{-1} \quad \text{and} \quad \boldsymbol{T}^{\mathbf{T}} = \left(\boldsymbol{H}^{-1}\right)^{\mathrm{T}} \boldsymbol{A}^{\mathbf{T}} \,.$$

But then

$$\boldsymbol{P} = \boldsymbol{T}\boldsymbol{T}^{\mathrm{T}} = \boldsymbol{A}\boldsymbol{H}^{-1} \left(\boldsymbol{H}^{-1}\right)^{\mathrm{T}} \boldsymbol{A}^{\mathrm{T}} = \boldsymbol{A} \left(\boldsymbol{H}^{\mathrm{T}}\boldsymbol{H}\right)^{-1} \boldsymbol{A}^{\mathrm{T}}$$

and as

$$\boldsymbol{H}^{\mathrm{T}}\boldsymbol{H} = \boldsymbol{A}^{\mathrm{T}}\boldsymbol{T}\boldsymbol{T}^{\mathrm{T}}\boldsymbol{A} = \boldsymbol{A}^{\mathrm{T}}\boldsymbol{P}\boldsymbol{A} = \boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$$

we finally arrive at

$$\boldsymbol{P} = \boldsymbol{A}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}. \tag{D.9}$$

Indeed, the so defined operator $\boldsymbol{P}$ accomplishes the orthogonal projection of $\boldsymbol{x}$ onto $R(\boldsymbol{A})$ in terms of the matrix $\boldsymbol{A}$ itself.

Let us add:

Consider an arbitrary vector $\boldsymbol{x}$ and conceive two different projection operators $\boldsymbol{P}_1$ and $\boldsymbol{P}_2$ producing likewise $\boldsymbol{P}_1\boldsymbol{x} = \boldsymbol{y}$ and $\boldsymbol{P}_2\boldsymbol{x} = \boldsymbol{y}$, respectively. In view of

$$(\boldsymbol{P}_1 - \boldsymbol{P}_2)\,\boldsymbol{x} = \boldsymbol{0}$$

the operators are identical. Put another way, the projection operator is unique.

The operator $\boldsymbol{P} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}$ is seen to be *idempotent*, $\boldsymbol{P}^2 = \boldsymbol{P}$, and symmetric, $\boldsymbol{P} = \boldsymbol{P}^{\mathrm{T}}$.

As has been discussed in Appendix A.2, in respect of $\mathrm{rank}(\boldsymbol{A}) = r$ we have $\mathrm{rank}(\boldsymbol{P}) = r$.

Let $\boldsymbol{v}$ be an eigenvector and $\lambda \neq 0$ an eigenvalue of $\boldsymbol{P}$, $\boldsymbol{P}\boldsymbol{v} = \lambda\boldsymbol{v}$. From

$$\boldsymbol{P}(\boldsymbol{P}\boldsymbol{v}) = \boldsymbol{P}(\lambda\boldsymbol{v}) = \lambda\boldsymbol{P}\boldsymbol{v} = \lambda^2\boldsymbol{v}$$

and

$$\boldsymbol{P}(\boldsymbol{P}\boldsymbol{v}) = \boldsymbol{P}^2\boldsymbol{v} = \boldsymbol{P}\boldsymbol{v} = \lambda\boldsymbol{v}$$

we draw $\lambda^2 = \lambda$ so that $\lambda = 1$. The eigenvalues of $\boldsymbol{P}$ are either 0 or 1.

As shown, e.g. in [59–61], the trace of $\boldsymbol{P}$ is given by the sum of its eigenvalues; further, the rank of $\boldsymbol{P}$ equals its trace. From this we take that r eigenvalues are 1 and the remaining $m - r$ are 0.

Appendix E
Least Squares Adjustments

Unconstrained Adjustment

Consider an $m \times r$ design matrix $\boldsymbol{A}$ of $\mathrm{rank}(\boldsymbol{A}) = r$. Due to measurement errors, the linear system

$$\boldsymbol{A}\boldsymbol{\beta} \approx \boldsymbol{x} \tag{E.1}$$

proves inconsistent, $\boldsymbol{x} \in V_m(\Re)$ and $\boldsymbol{A}\boldsymbol{\beta} \in V_m^r(\Re)$. Decomposing $V_m(\Re)$ into orthogonal subspaces $V_m^r(\Re)$ and $V_m^{m-r}(\Re)$ we have

$$V_m(\Re) = V_m^r(\Re) \oplus V_m^{m-r}(\Re) \; .$$

The method of least squares projects the vector $\boldsymbol{x}$ of observations orthogonally onto the subspace $V_m^r(\Re)$ so that $\boldsymbol{P}\boldsymbol{x} \in V_m^r(\Re)$. The projection via

$$\boldsymbol{P} = \boldsymbol{A}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}} \tag{E.2}$$

issues a vector of residuals $\bar{\boldsymbol{r}}$ satisfying $\boldsymbol{A}^{\mathbf{T}}\bar{\boldsymbol{r}} = \mathbf{0}$, $\bar{\boldsymbol{r}} \in V_m^{m-r}(\Re)$ and $\boldsymbol{x} - \bar{\boldsymbol{r}} = \boldsymbol{P}\boldsymbol{x} \in V_m^r(\Re)$. Ignoring $\bar{\boldsymbol{r}}$ and substituting $\boldsymbol{P}\boldsymbol{x}$ for $\boldsymbol{x}$,

$$\boldsymbol{A}\bar{\boldsymbol{\beta}} = \boldsymbol{P}\boldsymbol{x} \; , \tag{E.3}$$

the inconsistent system (E.1) becomes "solvable" in terms of least squares. This, indeed, is the quintessence of the proceeding—frankly speaking, a trick. Multiplying (E.3) on the left by $(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}$ yields the least squares estimator

$$\bar{\boldsymbol{\beta}} = \left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{x} \tag{E.4}$$

of the unknown true solution vector.

Constrained Adjustment

1. $\mathrm{rank}(\boldsymbol{A}) = r$

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Let the least squares estimator $\bar{\boldsymbol{\beta}}$ be required to exactly satisfy $q < r$ constraints

$$\boldsymbol{H}\bar{\boldsymbol{\beta}} = \boldsymbol{y}\,, \qquad \text{rank}(\boldsymbol{H}) = q\,. \tag{E.5}$$

Maintaining the idea of orthogonal projection, $\boldsymbol{P}\boldsymbol{x} \in V_m^r(\Re)$, the constraints ask us to look for an new projection operator, [56].

To this end, we initially conceive an auxiliary vector $\boldsymbol{\beta}^*$ evoking homogeneous constraints.[1] Be $\boldsymbol{\beta}^*$ any solution of (E.5),

$$\boldsymbol{H}\boldsymbol{\beta}^* = \boldsymbol{y}\,. \tag{E.6}$$

As β has not yet been fixed, we put

$$\boldsymbol{A}(\boldsymbol{\beta} - \boldsymbol{\beta}^*) \approx \boldsymbol{x} - \boldsymbol{A}\boldsymbol{\beta}^*\,, \quad \boldsymbol{H}(\boldsymbol{\beta} - \boldsymbol{\beta}^*) = \boldsymbol{0}\,.$$

With

$$\boldsymbol{\gamma} = \boldsymbol{\beta} - \boldsymbol{\beta}^*\,, \quad \boldsymbol{z} = \boldsymbol{x} - \boldsymbol{A}\boldsymbol{\beta}^* \tag{E.7}$$

we obtain the systems

$$\boldsymbol{A}\boldsymbol{\gamma} \approx \boldsymbol{z}\,, \quad \boldsymbol{H}\boldsymbol{\gamma} = \boldsymbol{0}\,. \tag{E.8}$$

Suppose that the projection operator, throwing $\boldsymbol{z}$ orthogonally onto the column space of $\boldsymbol{A}$, be known,

$$\boldsymbol{A}\bar{\boldsymbol{\gamma}} = \boldsymbol{P}\boldsymbol{z}\,. \tag{E.9}$$

We remind that now, as a matter of course, $\boldsymbol{P} \neq \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}$. Nevertheless, $\boldsymbol{P}\boldsymbol{z}$ has to be an element of the column space of $\boldsymbol{A}$. Solving for $\bar{\boldsymbol{\gamma}}$, we observe

$$\bar{\boldsymbol{\gamma}} = (\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{P}\boldsymbol{z}\,. \tag{E.10}$$

According to (E.8), we have

$$\boldsymbol{H}\bar{\boldsymbol{\gamma}} = \boldsymbol{H}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{P}\boldsymbol{z} = \boldsymbol{C}^{\mathrm{T}}\boldsymbol{P}\boldsymbol{z} = \boldsymbol{0}\,. \tag{E.11}$$

Hence, $\boldsymbol{P}\boldsymbol{z}$ has to be an element of the null space of the $(q \times m)$ matrix

$$\boldsymbol{C}^{\mathrm{T}} = \boldsymbol{H}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}\,.$$

After all, $\boldsymbol{P}\boldsymbol{z}$ is in the column space of $\boldsymbol{A}$ *and* in the null space of $\boldsymbol{C}^{\mathrm{T}}$,

$$\boldsymbol{P}\boldsymbol{z} \in R(\boldsymbol{A}) \cap N\left(\boldsymbol{C}^{\mathrm{T}}\right)\,.$$

The q linearly independent column vectors of the $(m \times q)$ matrix $\boldsymbol{C} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{H}^{\mathrm{T}}$ span a q-dimensional subspace $R(\boldsymbol{C}) = V_m^q(\Re)$ of the space $R(\boldsymbol{A}) = V_m^r(\Re)$, where $R(\boldsymbol{C}) \subset R(\boldsymbol{A})$. Furthermore

$$N(\boldsymbol{C}^{\mathrm{T}}) = V_m^{m-q}(\Re)\,, \quad R(\boldsymbol{C}) \perp N(\boldsymbol{C}^{\mathrm{T}}) \quad \text{and} \quad R(\boldsymbol{C}) \oplus N(\boldsymbol{C}^{\mathrm{T}}) = V_m(\Re)\,.$$

[1] The vector drops out later.

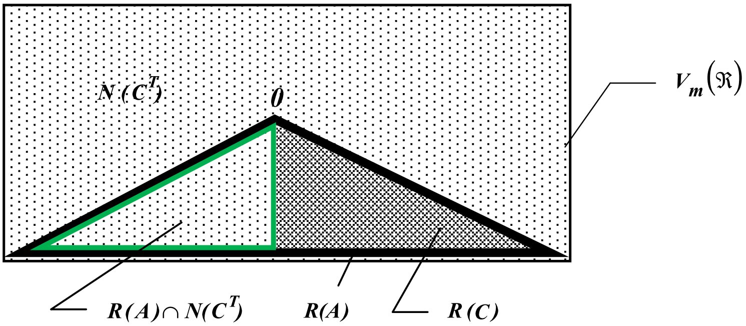

Fig. E.1 $V_m^r(\Re)$ symbolic, $R(\boldsymbol{C}) \subset R(\boldsymbol{A})$, $R(\boldsymbol{C}) \perp N(\boldsymbol{C}^{\mathrm{T}})$, intersection $R(\boldsymbol{A}) \cap N(\boldsymbol{C}^{\mathrm{T}})$

Figure E.1 depicts the intersection $R(\boldsymbol{A}) \cap N(\boldsymbol{C}^{\mathrm{T}})$ symbolically. To project onto just this intersection, we simply put

$$\begin{aligned}\boldsymbol{P} &= \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}} - \boldsymbol{C}(\boldsymbol{C}^{\mathrm{T}}\boldsymbol{C})^{-1}\boldsymbol{C}^{\mathrm{T}} \\ &= \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}} - \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{H}^{\mathrm{T}}[\boldsymbol{H}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{H}^{\mathrm{T}}]^{-1}\boldsymbol{H}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}\end{aligned}$$

so that the component of $\boldsymbol{z}$ being projected onto $R(\boldsymbol{C})$, $R(\boldsymbol{C}) \subset R(\boldsymbol{A})$ gets subtracted. Returning to $\bar{\boldsymbol{\beta}}$ via (E.7) yields

$$\bar{\boldsymbol{\beta}} - \boldsymbol{\beta}^* = (\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{P}(\boldsymbol{x} - \boldsymbol{A}\boldsymbol{\beta}^*)$$

or, due to (E.6),

$$\begin{aligned}\bar{\boldsymbol{\beta}} &= \left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{x} \\ &\quad - \left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{H}^{\mathrm{T}}\left[\boldsymbol{H}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{H}^{\mathrm{T}}\right]^{-1}\left[\boldsymbol{H}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{x} - \boldsymbol{y}\right].\end{aligned} \qquad \text{(E.12)}$$

Finally, we observe $\boldsymbol{H}\bar{\boldsymbol{\beta}} = \boldsymbol{y}$. The projection operator $\boldsymbol{P}$, as introduced ad hoc in (E.9), is seen to comprise two terms. Both effect orthogonal projections onto the column space of $\boldsymbol{A}$, though the second one is confined to an orthogonal projection onto the subspace $R(\boldsymbol{C}) \subset R(\boldsymbol{A})$. Also $(\boldsymbol{z} - \boldsymbol{P}\boldsymbol{z})^{\mathrm{T}}\boldsymbol{P}\boldsymbol{z} = \boldsymbol{0}$ as $\boldsymbol{P}^2 = \boldsymbol{P}$.

2. $\mathrm{rank}(\boldsymbol{A}) = r' < r$

We assume the first r' column vectors of the matrix $\boldsymbol{A}$ to be linearly independent. Then, partitioning the matrix $\boldsymbol{A}$ into an $(m \times r')$ matrix $\boldsymbol{A}_1$ and an $(m \times (r - r'))$ matrix $\boldsymbol{A}_2$ we have

$$\boldsymbol{A} = (\boldsymbol{A}_1 \,|\boldsymbol{A}_2)\ .$$

Ostensibly, the inconsistencies of the system (E.1) vanish, if the erroneous vector $\boldsymbol{x}$ is projected onto the column space of $\boldsymbol{A}_1$,

$$\boldsymbol{A}\,\bar{\boldsymbol{\beta}} = \boldsymbol{P}\boldsymbol{x}\,, \quad \boldsymbol{P} = \boldsymbol{A}_1\left(\boldsymbol{A}_1^{\mathrm{T}}\boldsymbol{A}_1\right)^{-1}\boldsymbol{A}_1^{\mathrm{T}}. \qquad \text{(E.13)}$$

However, as $\text{rank}(\boldsymbol{A}) = r' < r$, there are $q = (r - r')$ indeterminate components of the vector $\bar{\boldsymbol{\beta}}$. Consequently, we may add q constraints. As the column vectors $\boldsymbol{a}_k$; $k = r' + 1, \ldots, r$ are linear combinations of the column vectors $\boldsymbol{a}_k$; $k = 1, \ldots, r'$ and the projection of any vector lying in the column space of $\boldsymbol{A}_1$ gets reproduced, we have $\boldsymbol{P}\boldsymbol{A} = \boldsymbol{A}$ or $(\boldsymbol{P}\boldsymbol{A})^{\mathrm{T}} = \boldsymbol{A}^{\mathrm{T}}\boldsymbol{P} = \boldsymbol{A}^{\mathrm{T}}$. Hence, multiplying (E.13) on the left by $\boldsymbol{A}^{\mathrm{T}}$ yields

$$\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\bar{\boldsymbol{\beta}} = \boldsymbol{A}^{\mathrm{T}}\boldsymbol{x}\,. \tag{E.14}$$

Adding $q = r - r'$ constraints, we may solve the two systems simultaneously. To this end, we multiply (E.5) on left by $\boldsymbol{H}^{\mathrm{T}}$,

$$\boldsymbol{H}^{\mathrm{T}}\boldsymbol{H}\bar{\boldsymbol{\beta}} = \boldsymbol{H}^{\mathrm{T}}\boldsymbol{y} \tag{E.15}$$

so that

$$\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{H}\right)\bar{\boldsymbol{\beta}} = \boldsymbol{A}^{\mathrm{T}}\boldsymbol{x} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{y}\,. \tag{E.16}$$

Obviously, the auxiliary matrix

$$\boldsymbol{C} = \begin{pmatrix} \boldsymbol{A} \\ -- \\ \boldsymbol{H} \end{pmatrix}$$

possesses r' linearly independent rows in $\boldsymbol{A}$ and $q = r - r'$ linearly independent rows in $\boldsymbol{H}$ so that rank $(\boldsymbol{C}) = r$. Hence, the product matrix

$$\boldsymbol{C}^{\mathrm{T}}\boldsymbol{C} = \left(\boldsymbol{A}^{\mathbf{T}}\boldsymbol{A} + \boldsymbol{H}^{\mathbf{T}}\boldsymbol{H}\right)$$

is of rank r. Finally, (E.16) yields

$$\bar{\boldsymbol{\beta}} = \left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{H}\right)^{-1}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{x} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{y}\right)\,. \tag{E.17}$$

The two relationships [8],

$$\begin{aligned} \boldsymbol{H}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{H}\right)^{-1}\boldsymbol{A}^{\mathrm{T}} &= \boldsymbol{0} \\ \boldsymbol{H}\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} + \boldsymbol{H}^{\mathrm{T}}\boldsymbol{H}\right)^{-1}\boldsymbol{H}^{\mathrm{T}} &= \boldsymbol{I} \end{aligned} \tag{E.18}$$

in what $\boldsymbol{I}$ denotes a $(q \times q)$ identity matrix, reveals that $\bar{\boldsymbol{\beta}}$ indeed satisfies $\boldsymbol{H}\bar{\boldsymbol{\beta}} = \boldsymbol{y}$.

Appendix F
Expansion of Solution Vectors

Design matrices carrying erroneous entries may be tackled via series expansions.

Straight Lines

Section 13.4

Inserting the matrix elements

$$b_{i1} = \frac{1}{D}\left[\sum_{j=1}^{m}\bar{x}_j^2 - \bar{x}_i\sum_{j=1}^{m}\bar{x}_j\right],\ b_{i2} = \frac{1}{D}\left[-\sum_{j=1}^{m}\bar{x}_j + m\bar{x}_i\right];\quad i = 1,\ldots,m\,,$$

as given in (13.61), whereat

$$D = m\sum_{j=1}^{m}\bar{x}_j^2 - \left[\sum_{j=1}^{m}\bar{x}_j\right]^2,$$

into the least squares approach (13.58),

$$\bar{\beta}_k = \sum_{i=1}^{m} b_{ik}\,\bar{y}_i\,;\quad k = 1, 2\,,$$

we observe

$$\bar{\beta}_1 = \frac{1}{D}\left[\sum_{j=1}^{m}\bar{y}_j\sum_{j=1}^{m}\bar{x}_j^2 - \sum_{j=1}^{m}\bar{x}_j\,\bar{y}_j\sum_{j=1}^{m}\bar{x}_j\right]$$

and

$$\bar{\beta}_2 = \frac{1}{D}\left[-\sum_{j=1}^{m}\bar{x}_j\sum_{j=1}^{m}\bar{y}_j + m\sum_{j=1}^{m}\bar{x}_j\,\bar{y}_j\right].$$

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The quested derivatives c_{ik} take the form

$$c_{i1} = \frac{\partial \bar{\beta}_1}{\partial \bar{x}_i} = \frac{1}{D}\left[2\bar{x}_i \sum_{j=1}^{m} \bar{y}_j - \bar{y}_i \sum_{j=1}^{m} \bar{x}_j - \sum_{j=1}^{m} \bar{x}_j \bar{y}_j\right] - \frac{2\bar{\beta}_1}{D}\left[m\bar{x}_i - \sum_{j=1}^{m} \bar{x}_j\right]$$

$$c_{i+m,1} = \frac{\partial \bar{\beta}_1}{\partial \bar{y}_i} = \frac{1}{D}\left[\sum_{j=1}^{m} \bar{x}_j^2 - \bar{x}_i \sum_{j=1}^{m} \bar{x}_j\right]$$

$$c_{i2} = \frac{\partial \bar{\beta}_2}{\partial \bar{x}_i} = \frac{1}{D}\left[-\sum_{j=1}^{m} \bar{y}_j + m\bar{y}_i\right] - \frac{2\bar{\beta}_2}{D}\left[m\bar{x}_i - \sum_{j=1}^{m} \bar{x}_j\right]$$

$$c_{i+m,2} = \frac{\partial \bar{\beta}_2}{\partial \bar{y}_i} = \frac{1}{D}\left[-\sum_{j=1}^{m} \bar{x}_j + m\bar{x}_i\right]; \qquad i = 1, \ldots, m\,.$$

Summing over i reveals

$$\sum_{i=1}^{m} c_{i1} = -\bar{\beta}_2\,, \quad \sum_{i=1}^{m} c_{i+m,1} = 1\,, \quad \sum_{i=1}^{m} c_{i2} = 0\,, \quad \sum_{i=1}^{m} c_{i+m,2} = 0\,.$$

Planes

Section 15.4

The design matrix

$$\boldsymbol{A} = \begin{pmatrix} 1 & \bar{x}_1 & \bar{y}_1 \\ 1 & \bar{x}_2 & \bar{y}_2 \\ \cdots & \cdots & \cdots \\ 1 & \bar{x}_m & \bar{y}_m \end{pmatrix}$$

produces

$$\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} = \begin{pmatrix} H_{11} & H_{12} & H_{13} \\ H_{21} & H_{22} & H_{23} \\ H_{31} & H_{32} & H_{33} \end{pmatrix}$$

in what

$$H_{11} = m\,, \qquad H_{22} = \sum_{j=1}^{m} \bar{x}_j^2\,, \qquad H_{33} = \sum_{j=1}^{m} \bar{y}_j^2$$

$$H_{12} = H_{21} = \sum_{j=1}^{m} \bar{x}_j\,, \quad H_{13} = H_{31} = \sum_{j=1}^{m} \bar{y}_j\,, \quad H_{23} = H_{32} = \sum_{j=1}^{m} \bar{x}_j \bar{y}_j\,.$$

Further,

$$D = H_{11}\left(H_{22}H_{33} - H_{23}^2\right) + H_{12}\left(H_{31}H_{23} - H_{33}H_{12}\right) + H_{13}\left(H_{21}H_{32} - H_{13}H_{22}\right)$$

denotes the determinant of $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$. The inverse of $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$ reads

$$\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1} = \frac{1}{D}\begin{pmatrix} H_{22}H_{33} - H_{23}^2 & | \; H_{23}H_{13} - H_{12}H_{33} & | \; H_{12}H_{23} - H_{22}H_{13} \\ H_{23}H_{13} - H_{12}H_{33} \; | & H_{11}H_{33} - H_{13}^2 & | \; H_{12}H_{13} - H_{11}H_{23} \\ H_{12}H_{23} - H_{22}H_{13} \; | & H_{12}H_{13} - H_{11}H_{23} \; | & H_{11}H_{22} - H_{12}^2 \end{pmatrix}.$$

In view of $\boldsymbol{B} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}$, the components of $\bar{\boldsymbol{\beta}} = \boldsymbol{B}^{\mathrm{T}}\bar{\boldsymbol{z}}$ take the form

$$\bar{\beta}_1 = \sum_{j=1}^{m} b_{j1}\bar{z}_j\,, \qquad \bar{\beta}_2 = \sum_{j=1}^{m} b_{j2}\bar{z}_j\,, \qquad \bar{\beta}_3 = \sum_{j=1}^{m} b_{j3}\bar{z}_j\,,$$

in detail

$$\bar{\beta}_1 = \frac{1}{D}\sum_{j=1}^{m}\Big\{\Big[H_{22}H_{33} - H_{23}^2\Big] + \Big[H_{23}H_{13} - H_{12}H_{33}\Big]\bar{x}_j + \Big[H_{12}H_{23} - H_{22}H_{13}\Big]\bar{y}_j\Big\}\bar{z}_j$$

$$\bar{\beta}_2 = \frac{1}{D}\sum_{j=1}^{m}\Big\{\Big[H_{23}H_{13} - H_{12}H_{33}\Big] + \Big[H_{11}H_{33} - H_{13}^2\Big]\bar{x}_j + \Big[H_{12}H_{13} - H_{11}H_{23}\Big]\bar{y}_j\Big\}\bar{z}_j$$

$$\bar{\beta}_3 = \frac{1}{D}\sum_{j=1}^{m}\Big\{\Big[H_{12}H_{23} - H_{22}H_{13}\Big] + \Big[H_{12}H_{13} - H_{11}H_{23}\Big]\bar{x}_j + \Big[H_{11}H_{22} - H_{12}^2\Big]\bar{y}_j\Big\}\bar{z}_j\,.$$

The partial derivatives of the determinant are given by

$$\frac{\partial D}{\partial \bar{x}_i} = 2\Big[H_{11}H_{33} - H_{13}^2\Big]\bar{x}_i + 2\Big[H_{12}H_{13} - H_{11}H_{23}\Big]\bar{y}_i + 2\Big[H_{13}H_{23} - H_{12}H_{33}\Big]$$

$$\frac{\partial D}{\partial \bar{y}_i} = 2\Big[H_{12}H_{13} - H_{11}H_{23}\Big]\bar{x}_i + 2\Big[H_{11}H_{22} - H_{12}^2\Big]\bar{y}_i + 2\Big[H_{12}H_{23} - H_{13}H_{22}\Big]$$

$$\frac{\partial D}{\partial \bar{z}_i} = 0\,.$$

Differentiating each of the components $\bar{\beta}_k$; $k = 1, 2, 3$ with respect to x, y and z, we find

$$c_{i1} = \frac{\partial \bar{\beta}_1}{\partial \bar{x}_i} = -\frac{\bar{\beta}_1}{D}\frac{\partial D}{\partial \bar{x}_i} + \frac{1}{D}\left\{ 2\left(H_{33}\bar{x}_i - H_{23}\bar{y}_i\right)\sum_{j=1}^{m}\bar{z}_j + \left(H_{13}H_{23} - H_{12}H_{33}\right)\bar{z}_i + \left(H_{13}\bar{y}_i - H_{33}\right)\sum_{j=1}^{m}\bar{x}_j\bar{z}_j + \left(H_{23} + H_{12}\bar{y}_i - 2H_{13}\bar{x}_i\right)\sum_{j=1}^{m}\bar{y}_j\bar{z}_j \right\}$$

$$c_{i+m,1} = \frac{\partial \bar{\beta}_1}{\partial \bar{y}_i} = -\frac{\bar{\beta}_1}{D}\frac{\partial D}{\partial \bar{y}_i} + \frac{1}{D}\left\{ 2\left(H_{22}\bar{y}_i - H_{23}\bar{x}_i\right)\sum_{j=1}^{m}\bar{z}_j + \left(H_{12}H_{23} - H_{13}H_{22}\right)\bar{z}_i + \left(H_{23} + H_{13}\bar{x}_i - 2H_{12}\bar{y}_i\right)\sum_{j=1}^{m}\bar{x}_j\bar{z}_j + \left(H_{12}\bar{x}_i - H_{22}\right)\sum_{j=1}^{m}\bar{y}_j\bar{z}_j \right\}$$

$$c_{i+2m,1} = \frac{\partial \bar{\beta}_1}{\partial \bar{z}_i} = b_{i1}$$

$$c_{i2} = \frac{\partial \bar{\beta}_2}{\partial \bar{x}_i} = -\frac{\bar{\beta}_2}{D}\frac{\partial D}{\partial \bar{x}_i} + \frac{1}{D}\left\{ \left(H_{13}\bar{y}_i - H_{33}\right)\sum_{j=1}^{m}\bar{z}_j + \left(H_{11}H_{33} - H_{13}^2\right)\bar{z}_i + \left(H_{13} - H_{11}\bar{y}_i\right)\sum_{j=1}^{m}\bar{y}_j\bar{z}_j \right\}$$

$$c_{i+m,2} = \frac{\partial \bar{\beta}_2}{\partial \bar{y}_i} = -\frac{\bar{\beta}_2}{D}\frac{\partial D}{\partial \bar{y}_i} + \frac{1}{D}\left\{ \left(H_{23} + H_{13}\bar{x}_i - 2H_{12}\bar{y}_i\right)\sum_{j=1}^{m}\bar{z}_j + \left(H_{12}H_{13} - H_{11}H_{23}\right)\bar{z}_i + 2\left(H_{11}\bar{y}_i - H_{13}\right)\sum_{j=1}^{m}\bar{x}_j\bar{z}_j + \left(H_{12} - H_{11}\bar{x}_i\right)\sum_{j=1}^{m}\bar{y}_j\bar{z}_j \right\}$$

$$c_{i+2m,2} = \frac{\partial \bar{\beta}_2}{\partial \bar{z}_i} = b_{i2}$$

$$c_{i3} = \frac{\partial \bar{\beta}_3}{\partial \bar{x}_i} = -\frac{\bar{\beta}_3}{D}\frac{\partial D}{\partial \bar{x}_i} + \frac{1}{D}\left\{(H_{23} + H_{12}\bar{y}_i - 2H_{13}\bar{x}_i)\sum_{j=1}^{m}\bar{z}_j \right.$$
$$+ (H_{12}H_{13} - H_{11}H_{23})\,\bar{z}_i$$
$$\left. + \,(H_{13} - H_{11}\bar{y}_i)\sum_{j=1}^{m}\bar{x}_j\bar{z}_j + 2\,(H_{11}\bar{x}_i - H_{12})\sum_{j=1}^{m}\bar{y}_j\bar{z}_j\right\}$$

$$c_{i+m,3} = \frac{\partial \bar{\beta}_3}{\partial \bar{y}_i} = -\frac{\bar{\beta}_3}{D}\frac{\partial D}{\partial \bar{y}_i} + \frac{1}{D}\left\{(H_{12}\bar{x}_i - H_{22})\sum_{j=1}^{m}\bar{z}_j \right.$$
$$\left. + \left(H_{11}H_{22} - H_{12}^2\right)\bar{z}_i + (H_{12} - H_{11}\bar{x}_i)\sum_{j=1}^{m}\bar{x}_j\bar{z}_j\right\}$$

$$c_{i+2m,3} = \frac{\partial \bar{\beta}_3}{\partial \bar{z}_i} = b_{i3}\,.$$

Summation reveals

$$\sum_{i=1}^{m} c_{i1} = -\bar{\beta}_2\,, \qquad \sum_{i=1}^{m} c_{i+m,1} = -\bar{\beta}_3\,, \qquad \sum_{i=1}^{m} c_{i+2m,1} = 1$$
$$\sum_{i=1}^{m} c_{i2} = 0\,, \qquad \sum_{i=1}^{m} c_{i+m,2} = 0\,, \qquad \sum_{i=1}^{m} c_{i+2m,2} = 0$$
$$\sum_{i=1}^{m} c_{i3} = 0\,, \qquad \sum_{i=1}^{m} c_{i+m,3} = 0\,, \qquad \sum_{i=1}^{m} c_{i+2m,3} = 0\,.$$

Incidentally, in case of error-free x- and y-coordinates, as addressed in *Section 15.2*, (15.18), we easily prove

$$\sum_{i=1}^{m} b_{i1} = 1\,, \qquad \sum_{i=1}^{m} b_{i2} = 0\,, \qquad \sum_{i=1}^{m} b_{i3} = 0\,.$$

To this end, we have to substitute $x_{0,j}$ and $y_{0,j}$ for $\bar{x}_j$ and $\bar{y}_j$, respectively, hence to match matrix $\boldsymbol{A}$. Subsequently, just summations are asked for.

Circles

Section 16.2

Denoting

$$\boldsymbol{A} = \begin{pmatrix} 1 & \bar{u}_1 & \bar{v}_1 \\ 1 & \bar{u}_2 & \bar{v}_2 \\ \dots & \dots & \dots \\ 1 & \bar{u}_m & \bar{v}_m \end{pmatrix}$$

we have

$$A^{\mathrm{T}}A = \begin{pmatrix} H_{11} & H_{12} & H_{13} \\ H_{21} & H_{22} & H_{23} \\ H_{31} & H_{32} & H_{33} \end{pmatrix}$$

whereat

$$H_{11} = m\,, \qquad H_{22} = \sum_{j=1}^{m} \bar{u}_j^2\,, \qquad H_{33} = \sum_{j=1}^{m} \bar{v}_j^2$$

$$H_{12} = H_{21} = \sum_{j=1}^{m} \bar{u}_j\,, \quad H_{13} = H_{31} = \sum_{j=1}^{m} \bar{v}_j\,, \quad H_{23} = H_{32} = \sum_{j=1}^{m} \bar{u}_j \bar{v}_j\,.$$

The determinant of $A^{\mathrm{T}}A$ reads

$$D = H_{11}\left(H_{22}H_{33} - H_{23}^2\right) + H_{12}\left(H_{31}H_{23} - H_{33}H_{12}\right) + H_{13}\left(H_{21}H_{32} - H_{13}H_{22}\right)\,.$$

Further, we observe

$$\left(A^{\mathrm{T}}A\right)^{-1} = \frac{1}{D}\begin{pmatrix} H_{22}H_{33} - H_{23}^2 & | \; H_{23}H_{13} - H_{12}H_{33} & | \; H_{12}H_{23} - H_{22}H_{13} \\ H_{23}H_{13} - H_{12}H_{33} \; | & H_{11}H_{33} - H_{13}^2 & | \; H_{12}H_{13} - H_{11}H_{23} \\ H_{12}H_{23} - H_{22}H_{13} \; | & H_{12}H_{13} - H_{11}H_{23} \; | & H_{11}H_{22} - H_{12}^2 \end{pmatrix}.$$

Putting $B = A(A^{\mathrm{T}}A)^{-1}$, the components of $\bar{\beta} = B^{\mathrm{T}}\bar{w}$ take the form

$$\bar{\beta}_1 = \sum_{j=1}^{m} b_{j1}\bar{w}_j\,, \quad \bar{\beta}_2 = \sum_{j=1}^{m} b_{j2}\bar{w}_j\,, \quad \bar{\beta}_3 = \sum_{j=1}^{m} b_{j3}\bar{w}_j$$

or, detailed,

$$\bar{\beta}_1 = \frac{1}{D}\sum_{j=1}^{m}\Big\{\left[H_{22}H_{33} - H_{23}^2\right] + \left[H_{23}H_{13} - H_{12}H_{33}\right]\bar{u}_j + \left[H_{12}H_{23} - H_{22}H_{13}\right]\bar{v}_j\Big\}\bar{w}_j$$

$$\bar{\beta}_2 = \frac{1}{D}\sum_{j=1}^{m}\Big\{\left[H_{23}H_{13} - H_{12}H_{33}\right] + \left[H_{11}H_{33} - H_{13}^2\right]\bar{u}_j + \left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{v}_j\Big\}\bar{w}_j$$

$$\bar{\beta}_3 = \frac{1}{D}\sum_{j=1}^{m}\Big\{\left[H_{12}H_{23} - H_{22}H_{13}\right] + \left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{u}_j + \left[H_{11}H_{22} - H_{12}^2\right]\bar{v}_j\Big\}\bar{w}_j\,.$$

The partial derivatives of the determinant are given by

$$\frac{\partial D}{\partial \bar{x}_i} = \frac{2}{r^*}\Big[\Big(H_{11}H_{33} - H_{13}^2\Big)\,\bar{u}_i + (H_{13}H_{12} - H_{11}H_{23})\,\bar{v}_i + (H_{13}H_{23} - H_{33}H_{12})\Big]$$

$$\frac{\partial D}{\partial \bar{y}_i} = \frac{2}{r^*}\Big[(H_{12}H_{13} - H_{11}H_{23})\,\bar{u}_i + \Big(H_{11}H_{22} - H_{12}^2\Big)\,\bar{v}_i + (H_{12}H_{23} - H_{13}H_{22})\Big].$$

After all, we have

$$c_{i1} = \frac{\partial \bar{\beta}_1}{\partial \bar{x}_i} = -\frac{\bar{\beta}_1}{D}\frac{\partial D}{\partial \bar{x}_i} + \frac{1}{D}\Bigg\{\frac{2}{r^*}\,(H_{33}\bar{u}_i - H_{23}\bar{v}_i)\sum_{j=1}^{m}\bar{w}_j + \Big(H_{22}H_{33} - H_{23}^2\Big)\,\bar{u}_i + \frac{1}{r^*}\,(H_{13}\bar{v}_i - H_{33})\sum_{j=1}^{m}\bar{u}_j\bar{w}_j + (H_{23}H_{13} - H_{12}H_{33})\left(\frac{\bar{w}_i}{r^*} + \bar{u}_i^2\right) + \frac{1}{r^*}\,(H_{23} + H_{12}\bar{v}_i - 2H_{13}\bar{u}_i)\sum_{j=1}^{m}\bar{v}_j\bar{w}_j + (H_{12}H_{23} - H_{22}H_{13})\,\bar{u}_i\bar{v}_i\Bigg\}$$

$$c_{i+m,1} = \frac{\partial \bar{\beta}_1}{\partial \bar{y}_i} = -\frac{\bar{\beta}_1}{D}\frac{\partial D}{\partial \bar{y}_i} + \frac{1}{D}\Bigg\{\frac{2}{r^*}\,(H_{22}\bar{v}_i - H_{23}\bar{u}_i)\sum_{j=1}^{m}\bar{w}_j + \Big(H_{22}H_{33} - H_{23}^2\Big)\,\bar{v}_i + \frac{1}{r^*}\,(H_{13}\bar{u}_i + H_{23} - 2H_{12}\bar{v}_i)\sum_{j=1}^{m}\bar{u}_j\bar{w}_j + (H_{23}H_{13} - H_{12}H_{33})\,\bar{u}_i\bar{v}_i + \frac{1}{r^*}\,(H_{12}\bar{u}_i - H_{22})\sum_{j=1}^{m}\bar{v}_j\bar{w}_j + (H_{12}H_{23} - H_{22}H_{13})\left(\frac{\bar{w}_i}{r^*} + \bar{v}_i^2\right)\Bigg\}$$

$$c_{i2} = \frac{\partial \bar{\beta}_2}{\partial \bar{x}_i} = -\frac{\bar{\beta}_2}{D}\frac{\partial D}{\partial \bar{x}_i} + \frac{1}{D}\Bigg\{\frac{1}{r^*}\,(H_{13}\bar{v}_i - H_{33})\sum_{j=1}^{m}\bar{w}_j + (H_{23}H_{13} - H_{12}H_{33})\,\bar{u}_i + \Big(H_{11}H_{33} - H_{13}^2\Big)\left(\frac{\bar{w}_i}{r^*} + \bar{u}_i^2\right) + \frac{1}{r^*}\,(H_{13} + H_{11}\bar{v}_i)\sum_{j=1}^{m}\bar{v}_j\bar{w}_j + (H_{12}H_{13} - H_{11}H_{23})\,\bar{u}_i\bar{v}_i\Bigg\}$$

$$c_{i+m,2} = \frac{\partial \bar{\beta}_2}{\partial \bar{y}_i} = -\frac{\bar{\beta}_2}{D}\frac{\partial D}{\partial \bar{y}_i} + \frac{1}{D}\left\{\frac{1}{r^*}\left(H_{23} + H_{13}\bar{u}_i - 2H_{12}\bar{v}_i\right)\sum_{j=1}^{m}\bar{w}_j\right.$$

$$+ \left(H_{23}H_{13} - H_{12}H_{33}\right)\bar{v}_i$$

$$+ \frac{2}{r^*}\left(H_{11}\bar{v}_i - H_{13}\right)\sum_{j=1}^{m}\bar{u}_j\bar{w}_j + \left(H_{11}H_{33} - H_{13}^2\right)\bar{u}_i\bar{v}_i$$

$$\left. + \frac{1}{r^*}\left(H_{12} - H_{11}\bar{u}_i\right)\sum_{j=1}^{m}\bar{v}_j\bar{w}_j + \left(H_{12}H_{13} - H_{11}H_{23}\right)\left(\frac{\bar{w}_i}{r^*} + \bar{v}_i^2\right)\right\}$$

$$c_{i3} = \frac{\partial \bar{\beta}_3}{\partial \bar{x}_i} = -\frac{\bar{\beta}_3}{D}\frac{\partial D}{\partial \bar{x}_i} + \frac{1}{D}\left\{\frac{1}{r^*}\left(H_{23} + H_{12}\bar{v}_i - 2H_{13}\bar{u}_i\right)\sum_{j=1}^{m}\bar{w}_j\right.$$

$$+ \left(H_{12}H_{23} - H_{22}H_{13}\right)\bar{u}_i + \frac{1}{r^*}\left(H_{13} - H_{11}\bar{v}_i\right)\sum_{j=1}^{m}\bar{u}_j\bar{w}_j$$

$$+ \left(H_{12}H_{13} - H_{11}H_{23}\right)\left(\frac{\bar{w}_i}{r^*} + \bar{u}_i^2\right) + \frac{2}{r^*}\left(H_{11}\bar{u}_i - H_{12}\right)\sum_{j=1}^{m}\bar{v}_j\bar{w}_j$$

$$\left. + \left(H_{11}H_{22} - H_{12}^2\right)\bar{u}_i\bar{v}_i\right\}$$

$$c_{i+m,3} = \frac{\partial \bar{\beta}_3}{\partial \bar{y}_i} = -\frac{\bar{\beta}_3}{D}\frac{\partial D}{\partial \bar{y}_i} + \frac{1}{D}\left\{\frac{1}{r^*}\left(H_{12}\bar{u}_i - H_{22}\right)\sum_{j=1}^{m}\bar{w}_j\right.$$

$$+ \left(H_{12}H_{23} - H_{22}H_{13}\right)\bar{v}_i + \frac{1}{r^*}\left(H_{12} - H_{11}\bar{u}_i\right)\sum_{j=1}^{m}\bar{u}_j\bar{w}_j$$

$$\left. + \left(H_{12}H_{13} - H_{11}H_{23}\right)\bar{u}_i\bar{v}_i + \left(H_{11}H_{22} - H_{12}^2\right)\left(\frac{\bar{w}_i}{r^*} + \bar{v}_i^2\right)\right\}.$$

Section 16.3

The good news is that we may apply constitutive parts of *Section 15.4* by substituting ξ, η for x, y. Indeed, the design matrix

$$\boldsymbol{A} = \begin{pmatrix} 1 & \bar{\xi}_1 & \bar{\eta}_1 \\ 1 & \bar{\xi}_2 & \bar{\eta}_2 \\ \cdots & \cdots & \cdots \\ 1 & \bar{\xi}_m & \bar{\eta}_m \end{pmatrix}$$

leads to

$$\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} = \begin{pmatrix} H_{11} & H_{12} & H_{13} \\ H_{21} & H_{22} & H_{23} \\ H_{31} & H_{32} & H_{33} \end{pmatrix}$$

in which

$$H_{11} = m\,, \qquad H_{22} = \sum_{j=1}^{m} \bar{\xi}_j^2\,, \qquad H_{33} = \sum_{j=1}^{m} \bar{\eta}_j^2$$

$$H_{12} = H_{21} = \sum_{j=1}^{m} \bar{\xi}_j\,, \quad H_{13} = H_{31} = \sum_{j=1}^{m} \bar{\eta}_j\,, \quad H_{23} = H_{32} = \sum_{j=1}^{m} \bar{\xi}_j \bar{\eta}_j\,.$$

Let D denote the determinant of $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$,

$$D = H_{11}\left(H_{22}H_{33} - H_{23}^2\right) + H_{12}\left(H_{31}H_{23} - H_{33}H_{12}\right) + H_{13}\left(H_{21}H_{32} - H_{13}H_{22}\right)\,.$$

Furthermore, we observe

$$\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1} = \frac{1}{D}\begin{pmatrix} H_{22}H_{33} - H_{23}^2 & | \; H_{23}H_{13} - H_{12}H_{33} & | \; H_{12}H_{23} - H_{22}H_{13} \\ H_{23}H_{13} - H_{12}H_{33} & | \; H_{11}H_{33} - H_{13}^2 & | \; H_{12}H_{13} - H_{11}H_{23} \\ H_{12}H_{23} - H_{22}H_{13} & | \; H_{12}H_{13} - H_{11}H_{23} & | \; H_{11}H_{22} - H_{12}^2 \end{pmatrix}.$$

Putting $\boldsymbol{B} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}$, the components of $\bar{\boldsymbol{\beta}} = \boldsymbol{B}^{\mathrm{T}}\bar{\boldsymbol{\zeta}}$ take the form

$$\bar{\beta}_1 = \sum_{j=1}^{m} b_{j1}\bar{\zeta}_j\,, \quad \bar{\beta}_2 = \sum_{j=1}^{m} b_{j2}\bar{\zeta}_j\,, \quad \bar{\beta}_3 = \sum_{j=1}^{m} b_{j3}\bar{\zeta}_j$$

or, detailed,

$$\bar{\beta}_1 = \frac{1}{D}\sum_{j=1}^{m}\Big\{\left[H_{22}H_{33} - H_{23}^2\right] + \left[H_{23}H_{13} - H_{12}H_{33}\right]\bar{\xi}_j + \left[H_{12}H_{23} - H_{22}H_{13}\right]\bar{\eta}_j\Big\}\bar{\zeta}_j$$

$$\bar{\beta}_2 = \frac{1}{D}\sum_{j=1}^{m}\Big\{\left[H_{23}H_{13} - H_{12}H_{33}\right] + \left[H_{11}H_{33} - H_{13}^2\right]\bar{\xi}_j + \left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{\eta}_j\Big\}\bar{\zeta}_j$$

$$\bar{\beta}_3 = \frac{1}{D}\sum_{j=1}^{m}\Big\{\left[H_{12}H_{23} - H_{22}H_{13}\right] + \left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{\xi}_j + \left[H_{11}H_{22} - H_{12}^2\right]\bar{\eta}_j\Big\}\bar{\zeta}_j\,.$$

Looking for the partial derivatives of the $\bar{\beta}_k$; $k = 1, 2, 3$ with respect to x and y we invoke the chain rule

$$c_{ik} = \frac{\partial \bar{\beta}_k}{\partial \bar{x}_i} = \frac{\partial \bar{\beta}_k}{\partial \bar{\xi}_i}\frac{\partial \bar{\xi}_i}{\partial \bar{x}_i} + \frac{\partial \bar{\beta}_k}{\partial \bar{\eta}_i}\frac{\partial \bar{\eta}_i}{\partial \bar{x}_i} + \frac{\partial \bar{\beta}_k}{\partial \bar{\zeta}_i}\frac{\partial \bar{\zeta}_i}{\partial \bar{x}_i}\,; \quad i = 1, \ldots, m$$

$$c_{i+m,k} = \frac{\partial \bar{\beta}_k}{\partial \bar{y}_i} = \frac{\partial \bar{\beta}_k}{\partial \bar{\xi}_i}\frac{\partial \bar{\xi}_i}{\partial \bar{y}_i} + \frac{\partial \bar{\beta}_k}{\partial \bar{\eta}_i}\frac{\partial \bar{\eta}_i}{\partial \bar{y}_i} + \frac{\partial \bar{\beta}_k}{\partial \bar{\zeta}_i}\frac{\partial \bar{\zeta}_i}{\partial \bar{y}_i}\,; \quad k = 1, 2, 3$$

at what

$$\frac{\partial \bar{\xi}_i}{\partial \bar{x}_i} = 4R^2 \frac{4R^2 - \bar{x}_i^2 + \bar{y}_i^2}{(4R^2 + \bar{x}_i^2 + \bar{y}_i^2)^2}\,, \qquad \frac{\partial \bar{\xi}_i}{\partial \bar{y}_i} = -8R^2 \frac{\bar{x}_i\,\bar{y}_i}{(4R^2 + \bar{x}_i^2 + \bar{y}_i^2)^2}$$

$$\frac{\partial \bar{\eta}_i}{\partial \bar{x}_i} = -8R^2 \frac{\bar{x}_i\,\bar{y}_i}{(4R^2 + \bar{x}_i^2 + \bar{y}_i^2)^2}\,, \qquad \frac{\partial \bar{\eta}_i}{\partial \bar{y}_i} = 4R^2 \frac{4R^2 + \bar{x}_i^2 - \bar{y}_i^2}{(4R^2 + \bar{x}_i^2 + \bar{y}_i^2)^2}$$

$$\frac{\partial \bar{\zeta}_i}{\partial \bar{x}_i} = 16R^3 \frac{\bar{x}_i}{(4R^2 + \bar{x}_i^2 + \bar{y}_i^2)^2}\,, \qquad \frac{\partial \bar{\zeta}_i}{\partial \bar{y}_i} = 16R^3 \frac{\bar{y}_i}{(4R^2 + \bar{x}_i^2 + \bar{y}_i^2)^2}\,.$$

Further, we need the partial derivatives of the determinant D with respect to ξ and η,

$$\begin{aligned}
\frac{\partial D}{\partial \bar{\xi}_i} &= 2\left[H_{11}H_{33} - H_{13}^2\right]\bar{\xi}_i + 2\left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{\eta}_i \\
&\quad + 2\left[H_{13}H_{23} - H_{12}H_{33}\right] \\
\frac{\partial D}{\partial \bar{\eta}_i} &= 2\left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{\xi}_i + 2\left[H_{11}H_{22} - H_{12}^2\right]\bar{\eta}_i \\
&\quad + 2\left[H_{12}H_{23} - H_{13}H_{22}\right]\,.
\end{aligned}$$

Ultimately, the partial derivatives of the $\bar{\beta}_k$; $k = 1, 2, 3$ with respect to ξ and η read

$$\begin{aligned}
\frac{\partial \bar{\beta}_1}{\partial \bar{\xi}_i} &= -\frac{\bar{\beta}_1}{D}\frac{\partial D}{\partial \bar{\xi}_i} + \frac{1}{D}\Bigg[2(H_{33}\,\bar{\xi}_i - H_{23}\,\bar{\eta}_i)\sum_{j=1}^{m}\bar{\zeta}_j + (H_{13}H_{23} - H_{12}H_{33})\bar{\zeta}_i \\
&\quad + (H_{13}\,\bar{\eta}_i - H_{33})\sum_{j=1}^{m}\bar{\xi}_j\,\bar{\zeta}_j + (H_{23} + H_{12}\,\bar{\eta}_i - 2H_{13}\,\bar{\xi}_i)\sum_{j=1}^{m}\bar{\eta}_j\,\bar{\zeta}_j\Bigg] \\
\frac{\partial \bar{\beta}_1}{\partial \bar{\eta}_i} &= -\frac{\bar{\beta}_1}{D}\frac{\partial D}{\partial \bar{\eta}_i} + \frac{1}{D}\Bigg[2(H_{22}\,\bar{\eta}_i - H_{23}\,\bar{\xi}_i)\sum_{j=1}^{m}\bar{\zeta}_j + (H_{12}H_{23} - H_{13}H_{22})\,\bar{\zeta}_i \\
&\quad + (H_{23} + H_{13}\,\bar{\xi}_i - 2H_{12}\,\bar{\eta}_i)\sum_{j=1}^{m}\bar{\xi}_j\,\bar{\zeta}_j + (H_{12}\,\bar{\xi}_i - H_{22})\sum_{j=1}^{m}\bar{\eta}_j\,\bar{\zeta}_j\Bigg]
\end{aligned}$$

$$\frac{\partial \bar{\beta}_1}{\partial \bar{\zeta}_i} = b_{i1}$$

$$\frac{\partial \bar{\beta}_2}{\partial \bar{\xi}_i} = -\frac{\bar{\beta}_2}{D}\frac{\partial D}{\partial \bar{\xi}_i} + \frac{1}{D}\Bigg[(H_{13}\bar{\eta}_i - H_{33})\sum_{j=1}^{m}\bar{\zeta}_j + (H_{11}H_{33} - H_{13}^2)\bar{\zeta}_i + (H_{13} - H_{11}\bar{\eta}_i)\sum_{j=1}^{m}\bar{\eta}_j\bar{\zeta}_j\Bigg]$$

$$\frac{\partial \bar{\beta}_2}{\partial \bar{\eta}_i} = -\frac{\bar{\beta}_2}{D}\frac{\partial D}{\partial \bar{\eta}_i} + \frac{1}{D}\Bigg[(H_{23} + H_{13}\bar{\xi}_i - 2H_{12}\bar{\eta}_i)\sum_{j=1}^{m}\bar{\zeta}_j + (H_{12}H_{13} - H_{11}H_{23})\bar{\zeta}_i + 2(H_{11}\bar{\eta}_i - H_{13})\sum_{j=1}^{m}\bar{\xi}_j\bar{\zeta}_j + (H_{12} - H_{11}\bar{\xi}_i)\sum_{j=1}^{m}\bar{\eta}_j\bar{\zeta}_j\Bigg]$$

$$\frac{\partial \bar{\beta}_2}{\partial \bar{\zeta}_i} = b_{i2}$$

$$\frac{\partial \bar{\beta}_3}{\partial \bar{\xi}_i} = -\frac{\bar{\beta}_3}{D}\frac{\partial D}{\partial \bar{\xi}_i} + \frac{1}{D}\Bigg[(H_{23} + H_{12}\bar{\eta}_i - 2H_{13}\bar{\xi}_i)\sum_{j=1}^{m}\bar{\zeta}_j + (H_{12}H_{13} - H_{11}H_{23})\bar{\zeta}_i + (H_{13} - H_{11}\bar{\eta}_i)\sum_{j=1}^{m}\bar{\xi}_j\bar{\zeta}_j + 2(H_{11}\bar{\xi}_i - H_{12})\sum_{j=1}^{m}\bar{\eta}_j\bar{\zeta}_j\Bigg]$$

$$\frac{\partial \bar{\beta}_3}{\partial \bar{\eta}_i} = -\frac{\bar{\beta}_3}{D}\frac{\partial D}{\partial \bar{\eta}_i} + \frac{1}{D}\Bigg[(H_{12}\bar{\xi}_i - H_{22})\sum_{j=1}^{m}\bar{\zeta}_j + (H_{11}H_{22} - H_{12}^2)\bar{\zeta}_i + (H_{12} - H_{11}\bar{\xi}_i)\sum_{j=1}^{m}\bar{\xi}_j\bar{\zeta}_j\Bigg]$$

$$\frac{\partial \bar{\beta}_3}{\partial \bar{\zeta}_i} = b_{i3}\,.$$

Parabolas

Section 17.4

The design matrix

$$\boldsymbol{A} = \begin{pmatrix} 1 & \bar{x}_1 & \bar{x}_1^2 \\ 1 & \bar{x}_2 & \bar{x}_2^2 \\ \cdots & \cdots & \cdots \\ 1 & \bar{x}_m & \bar{x}_m^2 \end{pmatrix}$$

produces

$$\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A} = \begin{pmatrix} H_{11} & H_{12} & H_{13} \\ H_{21} & H_{22} & H_{23} \\ H_{31} & H_{32} & H_{33} \end{pmatrix}$$

whereat

$$H_{11} = m\,, \qquad H_{22} = \sum_{j=1}^{m} \bar{x}_j^2\,, \qquad H_{33} = \sum_{j=1}^{m} \bar{x}_j^4$$

$$H_{12} = H_{21} = \sum_{j=1}^{m} \bar{x}_j\,, \quad H_{13} = H_{31} = \sum_{j=1}^{m} \bar{x}_j^2\,, \quad H_{23} = H_{32} = \sum_{j=1}^{m} \bar{x}_j^3\,.$$

The determinant of $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$ reads

$$D = H_{11}\left(H_{22}H_{33} - H_{23}^2\right) + H_{12}\left(H_{31}H_{23} - H_{33}H_{12}\right) + H_{13}\left(H_{21}H_{32} - H_{13}H_{22}\right)\,.$$

Furthermore, we have

$$\left(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}\right)^{-1} = \frac{1}{D}\begin{pmatrix} H_{22}H_{33} - H_{23}^2 & | \; H_{23}H_{13} - H_{12}H_{33} & | \; H_{12}H_{23} - H_{22}H_{13} \\ H_{23}H_{13} - H_{12}H_{33} \; | & H_{11}H_{33} - H_{13}^2 & | \; H_{12}H_{13} - H_{11}H_{23} \\ H_{12}H_{23} - H_{22}H_{13} \; | & H_{12}H_{13} - H_{11}H_{23} \; | & H_{11}H_{22} - H_{12}^2 \end{pmatrix}\,.$$

Putting $\boldsymbol{B} = \boldsymbol{A}(\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A})^{-1}$ the components of $\bar{\boldsymbol{\beta}} = \boldsymbol{B}^{\mathrm{T}}\bar{\boldsymbol{y}}$ take the form

$$\bar{\beta}_1 = \sum_{j=1}^{m} b_{j1}\bar{y}_j\,, \quad \bar{\beta}_2 = \sum_{j=1}^{m} b_{j2}\bar{y}_j\,, \quad \bar{\beta}_3 = \sum_{j=1}^{m} b_{j3}\bar{y}_j$$

or, in detail,

$$\bar{\beta}_1 = \frac{1}{D}\sum_{j=1}^{m}\left\{\left[H_{22}H_{33} - H_{23}^2\right] + \left[H_{23}H_{13} - H_{12}H_{33}\right]\bar{x}_j + \left[H_{12}H_{23} - H_{22}H_{13}\right]\bar{x}_j^2\right\}\bar{y}_j$$

$$\bar{\beta}_2 = \frac{1}{D}\sum_{j=1}^{m}\left\{\left[H_{23}H_{13} - H_{12}H_{33}\right] + \left[H_{11}H_{33} - H_{13}^2\right]\bar{x}_j + \left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{x}_j^2\right\}\bar{y}_j$$

$$\bar{\beta}_3 = \frac{1}{D}\sum_{j=1}^{m}\left\{\left[H_{12}H_{23} - H_{22}H_{13}\right] + \left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{x}_j + \left[H_{11}H_{22} - H_{12}^2\right]\bar{x}_j^2\right\}\bar{y}_j\,.$$

The partial derivatives of the determinant turn out to be

$$\frac{\partial D}{\partial \bar{x}_i} = 2\left[H_{13}H_{23} - H_{12}H_{33}\right] + 2\left[H_{11}H_{33} + 2\left(H_{12}H_{23} - H_{13}H_{22}\right) - H_{13}^2\right]\bar{x}_i + 6\left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{x}_i^2 + 4\left(H_{11}H_{22} - H_{12}^2\right)\bar{x}_i^3$$

$$\frac{\partial D}{\partial \bar{y}_i} = 0\,.$$

Finally we observe

$$c_{i1} = \frac{\partial \bar{\beta}_1}{\partial \bar{x}_i} = -\frac{\bar{\beta}_1}{D}\frac{\partial D}{\partial \bar{x}_i} + \frac{1}{D}\left\{2\left(H_{33}\bar{x}_i - 3H_{23}\bar{x}_i^2 + 2H_{22}\bar{x}_i^3\right)\sum_{j=1}^{m}\bar{y}_j + \left(H_{23}H_{13} - H_{12}H_{33}\right)\bar{y}_i + \left(-H_{33} + 2H_{23}\bar{x}_i + 3H_{13}\bar{x}_i^2 - 4H_{12}\bar{x}_i^3\right)\sum_{j=1}^{m}\bar{x}_j\bar{y}_j + 2\left(H_{12}H_{23} - H_{22}H_{13}\right)\bar{x}_i\bar{y}_i + \left[H_{23} - 2\left(H_{13} + H_{22}\right)\bar{x}_i + 3H_{12}\bar{x}_i^2\right]\sum_{j=1}^{m}\bar{x}_j^2\bar{y}_j\right\}$$

$$c_{i+m,1} = \frac{\partial \bar{\beta}_1}{\partial \bar{y}_i} = b_{i1}$$

$$c_{i2} = \frac{\partial \bar{\beta}_2}{\partial \bar{x}_i} = -\frac{\bar{\beta}_2}{D}\frac{\partial D}{\partial \bar{x}_i} + \frac{1}{D}\left\{\left(-H_{33} + 2H_{23}\bar{x}_i + 3H_{13}\bar{x}_i^2 - 4H_{12}\bar{x}_i^3\right)\sum_{j=1}^{m}\bar{y}_j + 4\left(-H_{13}\bar{x}_i + H_{11}x_i^3\right)\sum_{j=1}^{m}\bar{x}_j\bar{y}_j + \left(H_{11}H_{33} - H_{13}^2\right)\bar{y}_i + 2\left(H_{12}H_{13} - H_{11}H_{23}\right)\bar{x}_i\bar{y}_i + \left[H_{13} + 2H_{12}\bar{x}_i - 3H_{11}\bar{x}_i^2\right]\sum_{j=1}^{m}\bar{x}_j^2\bar{y}_j\right\}$$

$$c_{i+m,2} = \frac{\partial \bar{\beta}_2}{\partial \bar{y}_i} = b_{i2}$$

$$c_{i3} = \frac{\partial \bar{\beta}_3}{\partial \bar{x}_i} = -\frac{\bar{\beta}_3}{D} \frac{\partial D}{\partial \bar{x}_i} + \frac{1}{D} \left\{ \left[H_{23} - 2\left(H_{13} + H_{22}\right)\bar{x}_i + 3H_{12}\bar{x}_i^2 \right] \sum_{j=1}^{m} \bar{y}_j \right.$$

$$+ \left(H_{13} + 2H_{12}\bar{x}_i - 3H_{11}\bar{x}_i^2 \right) \sum_{j=1}^{m} \bar{x}_j \bar{y}_j + \left(H_{12}H_{13} - H_{11}H_{23}\right)\bar{y}_i$$

$$\left. + \, 2\left(H_{11}H_{22} - H_{12}^2 \right) \bar{x}_i \bar{y}_i + 2\left(-H_{12} + H_{11}\bar{x}_i\right) \sum_{j=1}^{m} \bar{x}_j^2 \bar{y}_j \right\}$$

$$c_{i+m,3} = \frac{\partial \bar{\beta}_3}{\partial \bar{y}_i} = b_{i3} \, .$$

After all, summation over i discloses

$$\sum_{i=1}^{m} c_{i1} = -\bar{\beta}_2 \, , \qquad \sum_{i=1}^{m} c_{i+m,1} = 1$$

$$\sum_{i=1}^{m} c_{i2} = -2\bar{\beta}_3 \, , \qquad \sum_{i=1}^{m} c_{i+m,2} = 0$$

$$\sum_{i=1}^{m} c_{i3} = 0 \, , \qquad \sum_{i=1}^{m} c_{i+m,3} = 0 \, .$$

Appendix G
Student's Density

Suppose a random variable X to be $N(\mu, \sigma^2)$-distributed,

$$P\left(X \leq x\right) = \frac{1}{\sigma\sqrt{2\pi}} \int\limits_{-\infty}^{x} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) dx\,, \tag{G.1}$$

and assume n realizations

$$x_1, x_2, \ldots, x_n \tag{G.2}$$

of which to bring forth a sample variance

$$s^2 = \frac{1}{n-1}\sum_{l=1}^{n}(x_l - \bar{x})^2\;; \quad \nu = n-1\,. \tag{G.3}$$

Referring the upper integration limit to the center μ of the Gaussian density,

$$x = \mu + ts\,, \tag{G.4}$$

at what t denotes some real number, we have

$$P\left(X \leq \mu + ts\right) = \frac{1}{\sigma\sqrt{2\pi}} \int\limits_{-\infty}^{\mu+ts} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) dx\,. \tag{G.5}$$

Eventually, substituting $\eta = (x-\mu)/\sigma$ issues

$$P\left(X \leq \mu + ts\right) = P\left(t, s, \nu\right) = \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{ts/\sigma} \mathrm{e}^{-\eta^2/2} d\eta\,. \tag{G.6}$$

To render this statement statistically representative, we average by

$$p_{S^2}\left(s^2\right) = \frac{\nu^{\nu/2}}{2^{\nu/2}\Gamma\left(\nu/2\right)\sigma^{\nu}} \exp\left(-\frac{\nu s^2}{2\sigma^2}\right) s^{\nu-2} \tag{G.7}$$

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which we deduce from (3.27) putting

$$\chi^2 = (n-1)s^2/\sigma^2 \quad \text{and} \quad p_{S^2}(s^2) = p_{\chi^2} d\chi^2/ds^2 \, .$$

Incidentally, averaging by $p_S(s)$ leads to the same result since

$$p_S(s)ds = p_{S^2}(s^2)ds^2.$$

After all, we observe

$$P(t,\nu) = E\{P(t,s,\nu)\} = \int_0^\infty \left\{ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{ts/\sigma} \mathrm{e}^{-\eta^2/2} d\eta \right\} p_{S^2}\left(s^2\right) ds^2 \, . \qquad \text{(G.8)}$$

Obviously, (G.8) is a distribution function and its only variable is t. Differentiating with respect to t we observe

$$\begin{aligned} \frac{dP(t,\nu)}{dt} &= \int_0^\infty \left\{ \frac{s}{\sigma\sqrt{2\pi}} \exp\left(-\frac{t^2 s^2}{2\sigma^2}\right) \right\} p_{S^2}\left(s^2\right) ds^2 \\ &= \frac{\nu^{\nu/2}}{\sqrt{2\pi}\, 2^{\nu/2}\, \Gamma(\nu/2)\, \sigma^{\nu+1}} \int_0^\infty s^{\nu-1} \exp\left(-\frac{(t^2+\nu)s^2}{2\sigma^2}\right) ds^2. \end{aligned} \qquad \text{(G.9)}$$

Putting $\xi = s^2$; $d\xi = ds^2$ we take

$$\int_0^\infty \xi^{(\nu-1)/2} \exp\left(-\frac{(t^2+\nu)\xi}{2\sigma^2}\right) d\xi = \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\left(\frac{t^2+\nu}{2\sigma^2}\right)^{\frac{\nu+1}{2}}}$$

so that we indeed arrive at Student's (Gosset's) density

$$p_T(t,\nu) = \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\sqrt{\pi\nu}\;\Gamma\left(\frac{\nu}{2}\right)} \frac{1}{\left(1+\frac{t^2}{\nu}\right)^{\frac{\nu+1}{2}}} \, . \qquad \text{(G.10)}$$

According to (G.4), the underlying random variable

$$T(\nu) = \frac{X-\mu}{S} \qquad \text{(G.11)}$$

has $\nu = n-1$ degrees of freedom.

Instead of individual realization $x_1, x_2, \ldots, x_n$ of the random variable X, as addressed in (G.2), we now consider the arithmetic mean

$$\bar{x} = \frac{1}{n}\sum_{l=1}^{n} x_l \qquad \text{(G.12)}$$

and replace (G.4) by

$$\bar{x} = \mu + ts/\sqrt{n} \tag{G.13}$$

so that

$$P\left(\bar{X} \le \bar{x}\right) = \frac{1}{(\sigma/\sqrt{n})\,\sqrt{2\pi}} \int\limits_{-\infty}^{\bar{x}} \exp\left(-\frac{(\bar{x}-\mu)^2}{2\sigma^2/n}\right) d\bar{x} \tag{G.14}$$

or

$$P\left(\bar{X} \le \mu + ts/\sqrt{n}\right) = \frac{1}{(\sigma/\sqrt{n}\,)\,\sqrt{2\pi}} \int\limits_{-\infty}^{\mu+ts/\sqrt{n}} \exp\left(-\frac{(\bar{x}-\mu)^2}{2\sigma^2/n}\right) d\bar{x}\,. \tag{G.15}$$

Obviously, substituting $\eta = (\bar{x} - \mu)/(\sigma/\sqrt{n})$, reduces (G.15) to (G.6). Hence, the random variable

$$T(\nu) = \frac{\bar{X} - \mu}{S/\sqrt{n}} \tag{G.16}$$

is t-distributed with degrees of freedom $\nu = n - 1$.

Appendix H
Quantiles of Hotelling's Density

Table H.1 $t_{0.95}$; $P = 95$ %

$m/(n-1)$	1	2	3	4	5	6	7	8	9	10
1	13									
2	4.3	28								
3	3.2	7.6	44							
4	2.8	5.1	10.7	60						
5	2.6	4.2	6.8	13.9	76					
6	2.5	3.7	5.4	8.5	17.0	92				
7	2.4	3.5	4.8	6.7	10.3	20.1	108			
8	2.3	3.3	4.4	5.8	7.9	12.0	23.3	124		
9	2.3	3.2	4.1	5.2	6.7	9.1	13.7	26.4	140	
10	2.2	3.1	3.9	4.9	6.0	7.7	10.3	15.4	29.5	156
11	2.2	3.0	3.8	4.6	5.6	6.9	8.7	11.5	17.1	32.7
12	2.2	3.0	3.7	4.4	5.3	6.3	7.7	9.6	12.7	18.8
13	2.2	2.9	3.6	4.3	5.0	5.9	7.0	8.5	10.6	13.9
14	2.1	2.9	3.5	4.1	4.8	5.6	6.6	7.7	9.3	11.2
15	2.1	2.8	3.4	4.0	4.7	5.4	6.2	7.2	8.4	10.1
16	2.1	2.8	3.4	4.0	4.6	5.2	5.9	6.8	7.8	9.1
17	2.1	2.8	3.3	3.9	4.5	5.1	5.7	6.5	7.4	8.4
18	2.1	2.8	3.3	3.8	4.4	4.9	5.5	6.2	7.0	7.9
19	2.1	2.7	3.3	3.8	4.3	4.8	5.4	6.0	6.7	7.5
20	2.1	2.7	3.3	3.7	4.2	4.7	5.3	5.8	6.5	7.2
21	2.1	2.7	3.2	3.7	4.2	4.7	5.2	5.7	6.3	6.9
22	2.1	2.7	3.2	3.7	4.1	4.6	5.1	5.6	6.1	6.7
23	2.1	2.7	3.2	3.6	4.1	4.5	5.0	5.5	6.0	6.5
24	2.1	2.7	3.2	3.6	4.0	4.5	4.9	5.4	5.9	6.4
25	2.1	2.7	3.1	3.6	4.0	4.4	4.8	5.3	5.7	6.2
26	2.1	2.7	3.1	3.6	4.0	4.4	4.8	5.2	5.7	6.1
27	2.1	2.7	3.1	3.5	3.9	4.3	4.7	5.1	5.6	6.0
28	2.1	2.6	3.1	3.5	3.9	4.3	4.7	5.1	5.5	5.9
29	2.0	2.6	3.1	3.5	3.9	4.3	4.6	5.0	5.4	5.8
30	2.0	2.6	3.1	3.5	3.9	4.2	4.6	5.0	5.4	5.8
31		2.6	3.1	3.5	3.8	4.2	4.6	4.9	5.3	5.7
32			3.1	3.5	3.8	4.2	4.5	4.9	5.3	5.6
33				3.4	3.8	4.2	4.5	4.9	5.2	5.6
34					3.8	4.1	4.5	4.8	5.2	5.5
35						4.1	4.5	4.8	5.1	5.4
36							4.4	4.7	5.1	5.4
37								4.7	5.1	5.4
38									5.0	5.3
39										5.3

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Appendix I
Graphical Scale Transformations

We strive to graphically verify uncertainty assessments via data simulations.

Right from the start, we understand that the visualization of uncertainty intervals presents us with a pitfall: high-level metrology deals with relative uncertainties of the order of, say, 10^{-6} and less which the human eye is not in a position to resolve. Neither much coarser uncertainties of, say, 10^{-2} or 10^{-3} can be perceived visually. From there it suggests itself to resort to graphical expansion factors.

Mean Values

Let us start with the arithmetic mean and its uncertainty. Instead of

$$\bar{x} \pm u_{\bar{x}}$$

we depict

$$\bar{x} \pm u_{\bar{x}} V \, ; \qquad V \gg 1$$

with V an appropriate expansion factor. In a formal sense, we have to shift the true value x_0,

$$x_0^* = \bar{x} + (x_0 - \bar{x}) V \, . \tag{I.1}$$

Putting $V = 1$, we retrace $x_0^* = x_0$. Given

$$\bar{x} - u_{\bar{x}} V \leq x_0^* \leq \bar{x} + u_{\bar{x}} V \tag{I.2}$$

is fulfilled, the assessed uncertainty may be taken to be correct.

An equivalent transformation applies to the expectation $E\{\bar{X}\} = \mu_{\bar{x}}$ of the random variable $\bar{X}$. By means of the same expansion factor V, the confidence interval

$$\bar{x} \pm t_P \frac{s_x}{\sqrt{n}}$$

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passes into

$$\bar{x} \pm t_P \frac{s_x}{\sqrt{n}} V \,; \qquad V \gg 1$$

at what the formally shifted expectation takes the form

$$\mu_{\bar{x}}^* = \bar{x} + (\mu_{\bar{x}} - \bar{x})V \,. \tag{I.3}$$

Again, $V = 1$ recovers to $\mu_{\bar{x}}^* = \mu_{\bar{x}}$. The expanded confidence interval reads

$$\bar{x} - t_P \frac{s_x}{\sqrt{n}} V \le \mu_{\bar{x}}^* \le \bar{x} - t_P \frac{s_x}{\sqrt{n}} V \,.$$

Straight Lines

Assume the graph of the uncertainty band of a least squares line to be too narrow to be visually resolvable. Hence, instead of

$$\bar{y}(x) \pm u_{\bar{y}(x)}$$

we depict

$$\bar{y}(x) \pm V u_{\bar{y}(x)} \,; \qquad V \gg 1 \,. \tag{I.4}$$

The expansion prevents the two branches of the uncertainty region from pretendedly matching the fitted straight line

$$\bar{y}(x) = \bar{\beta}_1 + \bar{\beta}_2 x \,. \tag{I.5}$$

Obviously, the expansion of the uncertainty band asks us to formally readjust the position of the true straight line

$$y_0(x) = \beta_{0,1} + \beta_{0,2} x \,. \tag{I.6}$$

For some fixed x, any number lying in between $\bar{y}(x) - u_{\bar{y}(x)} \ldots \bar{y}(x) + u_{\bar{y}(x)}$ might be the true value $y_0(x)$. Hence, the true straight line is to be transformed according to

$$y_0^*(x) = \bar{y}(x) + \big(y_0(x) - \bar{y}(x)\big)V \,. \tag{I.7}$$

We observe that $V = 1$ reproduces $y_0^*(x) = y_0(x)$. Inserting (I.5) and (I.6), we have

$$\begin{aligned} y_0^*(x) &= \bar{\beta}_1 + \bar{\beta}_2 x + (\beta_{0,1} + \beta_{0,2} x - \bar{\beta}_1 - \bar{\beta}_2 x)V \\ &= [\,\bar{\beta}_1 + (\beta_{0,1} - \bar{\beta}_1)V\,] + [\,\bar{\beta}_2 + (\beta_{0,2} - \bar{\beta}_2)V\,]\,x \,. \end{aligned} \tag{I.8}$$

Thus, the coefficients of the formally transformed true straight line

$$y_0^*(x) = \beta_{0,1}^* + \beta_{0,2}^* x \tag{I.9}$$

read

$$\begin{aligned} \beta^*_{0,1} &= \bar{\beta}_1 + (\beta_{0,1} - \bar{\beta}_1)V \\ \beta^*_{0,2} &= \bar{\beta}_2 + (\beta_{0,2} - \bar{\beta}_2)V\,. \end{aligned} \tag{I.10}$$

To transform the expectations $E\{\bar{\beta}_1\} = \mu_{\bar{\beta}_1}$ and $E\{\bar{\beta}_2\} = \mu_{\bar{\beta}_2}$, we refer to the expectation of (I.5),

$$\mu_{\bar{y}(x)} = \mu_{\bar{\beta}_1} + \mu_{\bar{\beta}_2}\,x\,. \tag{I.11}$$

In view of (I.3) and (I.7) we have

$$\mu^*_{\bar{y}(x)} = \bar{y}(x) + (\mu_{\bar{y}(x)} - \bar{y}(x))V\,. \tag{I.12}$$

Thus, inserting (I.5) and (I.11), we observe

$$\begin{aligned} \mu^*_{\bar{\beta}_1} &= \bar{\beta}_1 + (\mu_{\bar{\beta}_1} - \bar{\beta}_1)V \\ \mu^*_{\bar{\beta}_2} &= \bar{\beta}_2 + (\mu_{\bar{\beta}_2} - \bar{\beta}_2)V\,. \end{aligned} \tag{I.13}$$

Planes

Instead of

$$\bar{z}(x, y) \pm u_{\bar{z}(x,y)}$$

the graph is to display

$$\bar{z}(x, y) \pm u_{\bar{z}(x,y)}V\,; \qquad V \gg 1\,. \tag{I.14}$$

By necessity, the expansion takes reference to the fitted plane

$$\bar{z}(x, y) = \bar{\beta}_1 + \bar{\beta}_2\,x + \bar{\beta}_3\,y\,. \tag{I.15}$$

Let us first transform the true plane

$$z_0(x, y) = \beta_{0,1} + \beta_{0,2}\,x + \beta_{0,3}\,y\,. \tag{I.16}$$

For some fixed point x, y, any number lying within $\bar{z}(x, y) - u_{\bar{z}(x,y)} \ldots \bar{z}(x, y) + u_{\bar{z}(x,y)}$ might be the true value $z(x_0, y_0)$. Hence,

$$z^*_0(x, y) = \bar{z}(x, y) + (z_0(x, y) - \bar{z}(x, y))V\,. \tag{I.17}$$

$V = 1$ reproduces $z^*_0(x, y) = z_0(x, y)$. Inserting (I.15) and (I.16) we find

$$\begin{aligned} z^*_0(x, y) &= \bar{\beta}_1 + \bar{\beta}_2\,x + \bar{\beta}_3\,y \\ &\quad + (\beta_{0,1} + \beta_{0,2}\,x + \beta_{0,3}\,y - \bar{\beta}_1 - \bar{\beta}_2\,x - \bar{\beta}_3\,y)V \\ &= [\,\bar{\beta}_1 + (\beta_{0,1} - \bar{\beta}_1)V\,] + [\,\bar{\beta}_2 + (\beta_{0,2} - \bar{\beta}_2)V\,]\,x \\ &\quad + [\,\bar{\beta}_3 + (\beta_{0,3} - \bar{\beta}_3)V\,]\,y\,. \end{aligned} \tag{I.18}$$

Thus, for the graphical purposes in view the true plane takes the form

$$z_0^*(x, y) = \beta_{0,1}^* + \beta_{0,2}^* x + \beta_{0,2}^* y \tag{I.19}$$

with coefficients

$$\begin{aligned} \beta_{0,1}^* &= \bar{\beta}_1 + (\beta_{0,1} - \bar{\beta}_1)V \\ \beta_{0,2}^* &= \bar{\beta}_2 + (\beta_{0,2} - \bar{\beta}_2)V \\ \beta_{0,3}^* &= \bar{\beta}_3 + (\beta_{0,3} - \bar{\beta}_3)V\,. \end{aligned} \tag{I.20}$$

To transform the expectations $E\{\bar{\beta}_1\} = \mu_{\bar{\beta}_1}$, $E\{\bar{\beta}_2\} = \mu_{\bar{\beta}_2}$ and $E\{\bar{\beta}_3\} = \mu_{\bar{\beta}_3}$ (I.15) tells us

$$\mu_{\bar{z}(x,y)} = \mu_{\bar{\beta}_1} + \mu_{\bar{\beta}_2} x + \mu_{\bar{\beta}_3} y\,. \tag{I.21}$$

But then

$$\mu_{\bar{z}(x,y)}^* = \bar{z}(x, y) + (\mu_{\bar{z}(x,y)} - \bar{z}(x, y))V \tag{I.22}$$

yields

$$\begin{aligned} \mu_{\bar{\beta}_1}^* &= \bar{\beta}_1 + (\mu_{\bar{\beta}_1} - \bar{\beta}_1)V \\ \mu_{\bar{\beta}_2}^* &= \bar{\beta}_2 + (\mu_{\bar{\beta}_2} - \bar{\beta}_2)V \\ \mu_{\bar{\beta}_3}^* &= \bar{\beta}_3 + (\mu_{\bar{\beta}_3} - \bar{\beta}_3)V\,. \end{aligned} \tag{I.23}$$

Parabolas

Instead of

$$\bar{y}(x) \pm u_{\bar{y}(x)}$$

the aim is to display

$$\bar{y}(x) \pm V u_{\bar{y}(x)}\,; \qquad V \gg 1 \tag{I.24}$$

letting the least squares parabola

$$\bar{y}(x) = \bar{\beta}_1 + \bar{\beta}_2 x + \bar{\beta}_3 x^2 \tag{I.25}$$

serve as a reference. The scale transformations shifts the true parabola

$$y_0(x) = \beta_{0,1} + \beta_{0,2} x + \beta_{0,3} x^2 \tag{I.26}$$

into

$$y_0^*(x) = \bar{y}(x) + (y_0(x) - \bar{y}(x))V \tag{I.27}$$

yielding

$$\begin{aligned} y_0^*(x) &= \bar{\beta}_1 + \bar{\beta}_2\,x + \bar{\beta}_3\,x^2 \\ &\quad + (\beta_{0,1} + \beta_{0,2}\,x + \beta_{0,3}\,x^2 - \bar{\beta}_1 - \bar{\beta}_2\,x - \bar{\beta}_3\,x^2)V \\ &= [\,\bar{\beta}_1 + (\beta_{0,1} - \bar{\beta}_1)V\,] + [\,\bar{\beta}_2 + (\beta_{0,2} - \bar{\beta}_2)V\,]\,x \\ &\quad + [\,\bar{\beta}_3 + (\beta_{0,3} - \bar{\beta}_3)V\,]\,x^2\,. \end{aligned} \tag{I.28}$$

Hence, the coefficients of the formally readjusted true parabola

$$y_0^*(x) = \beta_{0,1}^* + \beta_{0,2}^*\,x + \beta_{0,3}^*\,x^2 \tag{I.29}$$

turn out to be

$$\begin{aligned} \beta_{0,1}^* &= \bar{\beta}_1 + (\beta_{0,1} - \bar{\beta}_1)V \\ \beta_{0,2}^* &= \bar{\beta}_2 + (\beta_{0,2} - \bar{\beta}_2)V \\ \beta_{0,3}^* &= \bar{\beta}_3 + (\beta_{0,3} - \bar{\beta}_3)V\,. \end{aligned} \tag{I.30}$$

Finally, we transform the expectations $E\{\bar{\beta}_1\} = \mu_{\bar{\beta}_1}$, $E\{\bar{\beta}_2\} = \mu_{\bar{\beta}_2}$ and $E\{\bar{\beta}_3\} = \mu_{\bar{\beta}_3}$. Equation (I.25) produces

$$\mu_{\bar{y}(x)} = \mu_{\bar{\beta}_1} + \mu_{\bar{\beta}_2}\,x + \mu_{\bar{\beta}_3}\,x^2\,. \tag{I.31}$$

As

$$\mu_{\bar{y}(x)}^* = \bar{y}(x) + (\mu_{\bar{y}(x)} - \bar{y}(x))V \tag{I.32}$$

we find, inserting (I.25) and (I.31),

$$\begin{aligned} \mu_{\bar{\beta}_1}^* &= \bar{\beta}_1 + (\mu_{\bar{\beta}_1} - \bar{\beta}_1)V \\ \mu_{\bar{\beta}_2}^* &= \bar{\beta}_2 + (\mu_{\bar{\beta}_2} - \bar{\beta}_2)V \\ \mu_{\bar{\beta}_3}^* &= \bar{\beta}_3 + (\mu_{\bar{\beta}_3} - \bar{\beta}_3)V\,. \end{aligned} \tag{I.33}$$

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Index

A
Analysis of variance, 64
Arithmetic mean
  biased, 25
  uncertainty of, 69, 98
Arithmetic means
  compatibility of, 90
  difference between two, 61

B
Behrens–Fisher problem, 63
Bias
  controversy over, 73
  least squares solution vector, 124
  minimized sum of squares residuals, 127

C
Calibration chains, 323
Central limit theorem, 9
Check-weight, 324
Circles
  adjustment of, 245
  uncertainty region, 261
  via series expansion, 246
  via transformation, 252
Confidence ellipse and security polygon, merging of, 166
Confidence ellipsoid
  in least squares, 155
  practical, 49
Confidence ellipsoid and security polyhedron
  merging of, 169
Confidence interval, 31, 85
  in least squares, 142
Confidence level, 85
Consistency, 349
Conversion factor, 72
  uncertainty of, 78, 94
Correlation coefficient
  theoretical, 34
Covariance
  empirical, 39
    via Fisher's density, 45
  theoretical, 39
Covariance, composed, 109

D
Data transformation
  erroneous abscissas and erroneous ordinates, 298
Degrees of freedom, 37, 41
  effective, 63
Density of air, 9
Digits, significant, 14
Distribution, parent, 19
Distribution density
  chi-square, 37
  empirical, 18
  F, 40
  Fisher's, 44
  Hotelling's, 44, 47, 387
  Hotelling's, quantiles of, 51
  linear function of normal variables, 357
  multidimensional, normal, 35
  normal, 29
    convergence of, 31
    tails of, 31, 69
  standardized normal, 31
  Student's, 40, 383
  Student's, convergence of, 42
  theoretical, 18
  two-dimensional, normal, 33

M. Grabe, *Measurement Uncertainties in Science and Technology*,
DOI 10.1007/978-3-319-04888-8, © Springer-Verlag Berlin Heidelberg 2014

E
Ensemble, statistical, 54, 124
EP boundary, 164
EPC hull, 164
Error calculus, consistency of, 87
Error combination, arithmetic, 25
Error propagation, 26
  covering several stages, 105
Error propagation, series expansion, 81
Estimator, 4
  rounding of, 15
Example
  adjustment of a linear system, 148
  coefficient of thermal expansion, 201
  data transformation, 298
  Josephson effect, 13
  quantile of Hotelling's density, 52
  rounding of uncertainties, 14
  string of parabolas, 279
  traceability
    four measurands, one constant, 102
  weighted mean of means, 131
Expansion of solution vector
  circles, series expansion, 373
  circles, transformation, 376
  parabolas, 379
  planes, 370
  straight lines, 369
Expectation, 31
  arithmetic mean, 56
  empirical covariance, 60
  empirical variance, 57
  estimators, 54
Exponentials
  adjustment of, 203

F
Fairness, mutual, 12
Fundamental constants
  adjustment of, 337
  traceability of, 338
  uncertainties of, 347

G
Gauss–Markoff theorem, 129
  break down of, 129

H
Hotelling's density
  quantiles of, 387
Hotelling's ellipse, 48
Hotelling's ellipsoid, 49
Hypothesis testing, 31

I
Input data, consistency of, 132

K
Key comparisons, 314

L
Least squares
  constrained, 120, 279, 330, 366
  localization of true values, 131
  method of, 113
  points of attack, 130
  uncertainties, 131
  unconstrained, 116, 365
  weighted, 130

M
Mass decades, 324
Mass link-up
  constrained, 330
Matrix, rank of, 351
Mean of means
  non-weighted, 148
  uncertainty of, 147
  weighted, 144
Measurement
  art of, 6
  definition of, 3
  repeated, 10
  uncertainty of, 4
Measuring conditions
  well-defined, 38, 46
Measuring process, 11
  accuracy, 12
  precision, 12
  repeatability, 12
  reproducibility, 12
  stationary, 7

N
National metrology institutes, 12
Necessary and sufficient condition, 349

O
Outlier, 31

P
Pairwise comparisons, 329
Parabolas, adjustment of, 265
Physical constants, 86
Piecewise smooth approximation, 279
Planes, adjustment of, 217
Potato, convex, 164
  slice of, 164

Projection, orthogonal, 116, 361
Prototype, the kilogram, 323

R
Random errors, 9
origin of, 9
Random variables
sum of, 32, 36, 38, 43
Random variables, realization of, 18
Repeated measurements
uncertainty of, 69
Reproducibility, 73
Residuals
minimized sum of squared, 115
vector of, 114, 116
Resolving power, 18
Round robin, 91, 314

S
Scale transformations
graphical, 389
Security polygon, 156, 158
surfaces and lines of equal height, 163
Security polyhedron, 159
contour lines, 158
Security polytope, 163
Series expansion
truncation of, 82
SI units, 71
Standard
working, uncertainty of, 313
Standards
primary, 312
transfer, 314
working, 312
Straight line
transformation to, 209
Straight lines, adjustment of, 173
String of parabolas
uncertainty band of, 283
Systematic errors
accumulation in least squares, 147
confining intervals, 6
estimation of, 67
inconsistent propagation of, 107
of measurands, 80
propagation of, 136, 141
status of, 9

T
Traceability, 102, 319, 349
Trigonometric polynomial
adjustment of, 299
uncertainty band of, 304

U
Uncertainties
rounding of, 15
Uncertainties, test of via data simulation, 95
Uncertainty, 4
function of a measurand, 74
function of least squares estimators, 140, 150
function of several measurands, 81, 97
ppm, 13
relative, 13
Uncertainty spaces, 153
Unit
defined, 3
realized, 3

V
Variance–covariance matrix, 35
in least squares, 137, 141

W
Weighing scheme, 324
Weightings, consequences of, 143
Weights
arbitrary factor in, 131
varied by trial and error, 131