Part IX

Appendices

A Graphical Scale Transformations

The graphical visualization of uncertainty statements present us with a hitch. As we commonly assume relative uncertainties of, say, 10^{-3} and less, our eyes are not in a position to resolve the details. A way out is to introduce graphical expansion factors.

Mean Values

Let us graphically expand the uncertainty $u_{\bar{x}}$ of the arithmetic mean $\bar{x}$

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

To have a beneficial vista, instead of the metrologically defined result, we display

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

The factor V expands the primary uncertainty region with reference to the estimator $\bar{x}$. By means of data simulations, we constantly keep track of the true values of the measurands. Equation (A.1) tells us that any number lying within the expanded uncertainty region may symbolize the true value. Thus, in order to have a meaningful exposure the graph has, in a formal sense as a matter of course, to shift the true value x_0 of the mean $\bar{x}$ according to

$$x_0^* = \bar{x} + (x_0 - \bar{x})V \,; \qquad V \gg 1 \tag{A.2}$$

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

A similar transformation applies to the expectation $E\{\bar{X}\} = \mu_{\bar{x}}$ of the random variable $\bar{X}$

$$\mu_{\bar{x}}^* = \bar{x} + (\mu_{\bar{x}} - \bar{x})V \,; \qquad V \gg 1 \,. \tag{A.3}$$

Again, $V = 1$ recovers $\mu_{\bar{x}}^* = \mu_{\bar{x}}$.

Straight Lines

Assume the graphical display of the uncertainty band of a least squares line to be too narrow to be visually resolved. Hence, instead of

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

we depict

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

The expansion prevents the two branches of the uncertainty region to pretendedly match the fitted straight line

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

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

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

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

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

Obviously, $V = 1$ yields $y_0^*(x) = y_0(x)$. Inserting (A.5) and (A.6), we have

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

Hence, we display the true straight line following

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

with coefficients

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

To transform the expectations $E\{\bar{\beta}_1\} = \mu_{\bar{\beta}_1}$ and $E\{\bar{\beta}_2\} = \mu_{\bar{\beta}_2}$, we start from (A.5)

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

Equation (A.7) tells us

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

Thus, inserting (A.5) and (A.11), we find

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

Planes

Instead of

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

the diagram is intended to display

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

By necessity, the expansion has to take reference to the fitted plane

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

Initially, we readjust the true plane

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

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

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

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

$$\begin{aligned} z_0^*(x,y) &= \bar{\beta}_1 + \bar{\beta}_2\, x + \bar{\beta}_3\, y \\ &\quad + (\beta_{0,1} + \beta_{0,2}\, x + \beta_{0,3}\, y - \bar{\beta}_1 - \bar{\beta}_2\, x - \bar{\beta}_3\, y)V \\ &= [\,\bar{\beta}_1 + (\beta_{0,1} - \bar{\beta}_1)V\,] + [\,\bar{\beta}_2 + (\beta_{0,2} - \bar{\beta}_2)V\,]\, x \\ &\quad + [\,\bar{\beta}_3 + (\beta_{0,3} - \bar{\beta}_3)V\,]\, y\,. \end{aligned} \tag{A.18}$$

Thus, for graphical ends the true plane reads

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

with coefficients

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

We also transform the expectations $E\{\bar{\beta}_1\} = \mu_{\bar{\beta}_1}$, $E\{\bar{\beta}_2\} = \mu_{\bar{\beta}_2}$ and $E\{\bar{\beta}_3\} = \mu_{\bar{\beta}_3}$. From (A.15) we take

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

But then

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

yields

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

Parabolas

Instead of

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

we wish to display

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

where the least squares parabola

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

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

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

into

$$y^*_0(x) = \bar{y}(x) + (y_0(x) - \bar{y}(x))V \tag{A.27}$$

yielding

$$\begin{aligned}y^*_0(x) &= \bar{\beta}_1 + \bar{\beta}_2\,x + \bar{\beta}_3\,x^2\\ &\quad + (\beta_{0,1} + \beta_{0,2}\,x + \beta_{0,3}\,x^2 - \bar{\beta}_1 - \bar{\beta}_2\,x - \bar{\beta}_3\,x^2)V\\ &= [\,\bar{\beta}_1 + (\beta_{0,1} - \bar{\beta}_1)V\,] + [\,\bar{\beta}_2 + (\beta_{0,2} - \bar{\beta}_2)V\,]\,x\\ &\quad + [\,\bar{\beta}_3 + (\beta_{0,3} - \bar{\beta}_3)V,]\,x^2\,.\end{aligned} \tag{A.28}$$

Hence, the coefficients of the readjusted true parabola

$$y^*_0(x) = \beta^*_{0,1} + \beta^*_{0,2}\,x + \beta^*_{0,3}\,x^2 \tag{A.29}$$

turn out to be

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

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

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

As

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

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

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

B Expansion of Solution Vectors

Given the abscissas as well as ordinates are considered erroneous, the fitting of geometrical objects implies erroneous design matrices. Then, error propagation requires us to carry out series expansions of the solution vectors.

Straight Lines – Section 15.3

The series expansions of the components $\bar{\beta}_1$, $\bar{\beta}_2$ produce coefficients

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

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

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

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

For convenience, the coefficients have been gathered within an auxiliary matrix as stated in (15.9).

Planes – Section 19.3

The design matrix

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

produces

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

with elements

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

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

Let

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

denote the determinant of $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$. With this, the inverse of $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$ reads

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

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

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

more detailed

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

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

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

The partial derivatives of the determinant are issued as

$$\frac{\partial D}{\partial \bar{x}_i} = 2\left[H_{11}H_{33} - H_{13}^2\right]\bar{x}_i + 2\left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{y}_i$$
$$+2\left[H_{13}H_{23} - H_{12}H_{33}\right]$$
$$\frac{\partial D}{\partial \bar{y}_i} = 2\left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{x}_i + 2\left[H_{11}H_{22} - H_{12}^2\right]\bar{y}_i$$
$$+2\left[H_{12}H_{23} - H_{13}H_{22}\right]$$
$$\frac{\partial D}{\partial \bar{z}_i} = 0\,.$$

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

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

$$c_{i+m,1} = \frac{\partial \bar{\beta}_1}{\partial \bar{y}_i} = -\frac{\bar{\beta}_1}{D}\frac{\partial D}{\partial \bar{y}_i}$$
$$+\frac{1}{D}\left\{2\left(H_{22}\bar{y}_i - H_{23}\bar{x}_i\right)\sum_{j=1}^{m}\bar{z}_j + \left(H_{12}H_{23} - H_{13}H_{22}\right)\bar{z}_i\right.$$
$$\left. + \left(H_{23} + H_{13}\bar{x}_i - 2H_{12}\bar{y}_i\right)\sum_{j=1}^{m}\bar{x}_j\bar{z}_j + \left(H_{12}\bar{x}_i - H_{22}\right)\sum_{j=1}^{m}\bar{y}_j\bar{z}_j\right\}$$
$$c_{i+2m,1} = \frac{\partial \bar{\beta}_1}{\partial \bar{z}_i} = b_{i1}$$
$$c_{i2} = \frac{\partial \bar{\beta}_2}{\partial \bar{x}_i} = -\frac{\bar{\beta}_2}{D}\frac{\partial D}{\partial \bar{x}_i} + \frac{1}{D}\left\{\left(H_{13}\bar{y}_i - H_{33}\right)\sum_{j=1}^{m}\bar{z}_j\right.$$
$$\left. + \left(H_{11}H_{33} - H_{13}^2\right)\bar{z}_i + \left(H_{13} - H_{11}\bar{y}_i\right)\sum_{j=1}^{m}\bar{y}_j\bar{z}_j\right\}$$

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

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

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

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

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

$$+ (H_{12}H_{13} - H_{11}H_{23})\,\bar{z}_i$$

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

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

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

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

Parabolas – Section 23.4

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

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

with elements

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

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

Denoting the determinant of $\boldsymbol{A}^{\mathrm{T}}\boldsymbol{A}$ by

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

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

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

i.e.

$$\begin{aligned} \bar{\beta}_1 &= \frac{1}{D}\sum_{j=1}^{m}\left\{\left[H_{22}H_{33} - H_{23}^2\right] + \left[H_{23}H_{13} - H_{12}H_{33}\right]\bar{x}_j \right. \\ &\quad \left. + \left[H_{12}H_{23} - H_{22}H_{13}\right]\bar{x}_j^2\right\}\bar{y}_j \\ \bar{\beta}_2 &= \frac{1}{D}\sum_{j=1}^{m}\left\{\left[H_{23}H_{13} - H_{12}H_{33}\right] + \left[H_{11}H_{33} - H_{13}^2\right]\bar{x}_j \right. \\ &\quad \left. + \left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{x}_j^2\right\}\bar{y}_j \\ \bar{\beta}_3 &= \frac{1}{D}\sum_{j=1}^{m}\left\{\left[H_{12}H_{23} - H_{22}H_{13}\right] + \left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{x}_j \right. \\ &\quad \left. + \left[H_{11}H_{22} - H_{12}^2\right]\bar{x}_j^2\right\}\bar{y}_j\,. \end{aligned}$$

The partial derivatives of the determinant turn out to be

$$\begin{aligned} \frac{\partial D}{\partial \bar{x}_i} &= 2\left[H_{13}H_{23} - H_{12}H_{33}\right] \\ &\quad + 2\left[H_{11}H_{33} + 2\left(H_{12}H_{23} - H_{13}H_{22}\right) - H_{13}^2\right]\bar{x}_i \\ &\quad + 6\left[H_{12}H_{13} - H_{11}H_{23}\right]\bar{x}_i^2 + 4\left(H_{11}H_{22} - H_{12}^2\right)\bar{x}_i^3 \\ \frac{\partial D}{\partial \bar{y}_i} &= 0\,. \end{aligned}$$

Those of the components of the solution vector read

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

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

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

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

$$c_{i3} = \frac{\partial \bar{\beta}_3}{\partial \bar{x}_i} = -\frac{\bar{\beta}_3}{D}\frac{\partial D}{\partial \bar{x}_i} + \frac{1}{D}\left\{ \left[H_{23} - 2\left(H_{13} + H_{22}\right)\bar{x}_i + 3H_{12}\bar{x}_i^2\right]\sum_{j=1}^{m}\bar{y}_j \right.$$
$$+ \left(H_{13} + 2H_{12}\bar{x}_i - 3H_{11}\bar{x}_i^2\right)\sum_{j=1}^{m}\bar{x}_j\bar{y}_j + \left(H_{12}H_{13} - H_{11}H_{23}\right)\bar{y}_i$$
$$\left. +2\left(H_{11}H_{22} - H_{12}^2\right)\bar{x}_i\bar{y}_i + 2\left(-H_{12} + H_{11}\bar{x}_i\right)\sum_{j=1}^{m}\bar{x}_j^2\bar{y}_j \right\}$$

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

C Special Confidence Ellipses and Ellipsoids

In case repeated measurements are lacking, confidence ellipses and ellipsoids are not ready to hand. In the following, a heuristic approach is discussed.

Ellipses

Chapter 13 relates the adjustment of a straight line to individual measurements. In order to design a confidence ellipse, we start from Hotelling's ellipse as given, e.g., in (3.71), [28]

$$\begin{aligned} t^2(2,n-1) &= n(\bar{\boldsymbol{\zeta}}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{s}^{-1}(\bar{\boldsymbol{\zeta}}-\boldsymbol{\mu}) \\ &= \frac{n}{|\boldsymbol{s}\,|}\left[s_{yy}(\bar{x}-\mu_x)^2 - 2s_{xy}(\bar{x}-\mu_x)(\bar{y}-\mu_y) + s_{xx}(\bar{y}-\mu_y)^2\right] . \end{aligned} \tag{C.1}$$

Putting

$$\bar{\boldsymbol{s}}^{-1} = n\boldsymbol{s}^{-1}$$

where

$$\boldsymbol{s} = \begin{pmatrix} s_{xx} & s_{xy} \\ s_{yx} & s_{yy} \end{pmatrix} ; \qquad \bar{\boldsymbol{s}} = \begin{pmatrix} \dfrac{s_{xx}}{n} & \dfrac{s_{xy}}{n} \\ \dfrac{s_{yx}}{n} & \dfrac{s_{yy}}{n} \end{pmatrix} \tag{C.2}$$

we have

$$\begin{aligned} t^2(2,n-1) &= (\bar{\boldsymbol{\zeta}}-\boldsymbol{\mu})^{\mathrm{T}}\bar{\boldsymbol{s}}^{-1}(\bar{\boldsymbol{\zeta}}-\boldsymbol{\mu}) \\ &= \frac{1}{|\bar{\boldsymbol{s}}\,|}\left[\frac{s_{yy}}{n}(\bar{x}-\mu_x)^2 - 2\frac{s_{xy}}{n}(\bar{x}-\mu_x)(\bar{y}-\mu_y) + \frac{s_{xx}}{n}(\bar{y}-\mu_y)^2\right] . \end{aligned} \tag{C.3}$$

To recall, the ellipse refers to arithmetic means $\bar{x}$, $\bar{y}$ with expectations μ_x, μ_y and an empirical variance–covariance matrix $\bar{\boldsymbol{s}}$, the elements of which have degrees of freedom $n-1$.

By contrast, Sect. 13.6 considers estimators $\bar{\beta}_1$, $\bar{\beta}_2$ with expectations $\mu_{\bar{\beta}_1}$ and $\mu_{\bar{\beta}_2}$ and empirical variance–covariance matrix

$$\boldsymbol{s}_{\bar{\boldsymbol{\beta}}} = \begin{pmatrix} s_{\bar{\beta}_1\bar{\beta}_1} & s_{\bar{\beta}_1\bar{\beta}_2} \\ s_{\bar{\beta}_2\bar{\beta}_1} & s_{\bar{\beta}_2\bar{\beta}_2} \end{pmatrix} \tag{C.4}$$

the elements of which have degrees of freedom $m - 2$.

Let us tentatively cast Hotelling's ellipse into

$$\begin{aligned} t^2(2,\ldots) &= (\bar{\boldsymbol{\beta}} - \boldsymbol{\mu}_{\bar{\boldsymbol{\beta}}})^{\mathrm{T}} s_{\bar{\boldsymbol{\beta}}}^{-1} (\bar{\boldsymbol{\beta}} - \boldsymbol{\mu}_{\bar{\boldsymbol{\beta}}}) \\ &= \frac{1}{|\boldsymbol{s}_{\bar{\boldsymbol{\beta}}}|} \left[s_{\bar{\beta}_2\bar{\beta}_2} (\bar{\beta}_1 - \mu_{\bar{\beta}_1})^2 - 2 s_{\bar{\beta}_1\bar{\beta}_2} (\bar{\beta}_1 - \mu_{\bar{\beta}_1})(\bar{\beta}_2 - \mu_{\bar{\beta}_2}) \right. \\ &\quad \left. + \; s_{\bar{\beta}_1\bar{\beta}_1} (\bar{\beta}_2 - \mu_{\bar{\beta}_2})^2 \right] . \end{aligned} \tag{C.5}$$

While (C.3) includes repeated measurements (C.5) does not. Nevertheless, in both cases, the statistical fluctuations per se stand on an equal footing. To invoke the pertaining density a formal n is needed.

Hotelling's density reads

$$\begin{aligned} & p_T(t; m, n-1) \\ &= \frac{2\Gamma(n/2)}{(n-1)^{m/2}\Gamma[(n-m)/2]\Gamma(m/2)} \frac{t^{m-1}}{[1 + t^2/(n-1)]^{n/2}} \\ & t > 0\,, \quad n > m \end{aligned} \tag{C.6}$$

Let us firstly substitute the number 2 for m as we are considering two variables,

$$p_T(t; 2, n-1) = \frac{2\Gamma(n/2)}{(n-1)\Gamma[(n-2)/2]} \frac{t}{[1 + t^2/(n-1)]^{n/2}} \,.$$

Next we replace Hotelling's degrees of freedom $n-1$ by the degrees of freedom of the elements of the matrix (C.4), i.e. by $m - 2$. Hence

$$p_T(t; 2, m-2) = \frac{2\Gamma((m-1)/2)}{(m-2)\Gamma[(m-3)/2]} \frac{t}{[1 + t^2/(m-2)]^{(m-1)/2}} \,. \tag{C.7}$$

After all, the proceeding suggests to assign the confidence ellipse

$$\begin{aligned} & s_{\bar{\beta}_2\bar{\beta}_2} (\beta_1 - \bar{\beta}_1)^2 - 2 s_{\bar{\beta}_1\bar{\beta}_2} (\beta_1 - \bar{\beta}_1)(\beta_2 - \bar{\beta}_2) + s_{\bar{\beta}_1\bar{\beta}_1} (\beta_2 - \bar{\beta}_2)^2 \\ & = t_P^2(2, m-2) |\boldsymbol{s}_{\bar{\boldsymbol{\beta}}}| \end{aligned} \tag{C.8}$$

to the empirical estimators $\bar{\beta}_1, \bar{\beta}_2$ of the adjustment of a straight line as discussed in Chap. 13. Consulting a table for the quantiles of Hotelling's density, we look for the entry which refers to 2 variables and $m-2$ degrees of freedom. After all, we expect (C.8) to localize the point

$$\boldsymbol{\mu}_{\bar{\boldsymbol{\beta}}} = \begin{pmatrix} \mu_{\bar{\beta}_1} \\ \\ \mu_{\bar{\beta}_2} \end{pmatrix} \tag{C.9}$$

with probability P.

Finally, we hint that the ellipse's angle of rotation

$$\tan(2\varphi) = \frac{-s_{\bar{\beta}_1\bar{\beta}_2}}{s_{\bar{\beta}_2\bar{\beta}_2} - s_{\bar{\beta}_1\bar{\beta}_1}}\,, \tag{C.10}$$

measured counterclockwise against the β_1-axis of a rectangular β_1, β_2-coordinate system, proves sample-independent as the empirical variance s_y^2 cancels out.

Ellipsoids

Chapter 17 relates the adjustment of a plane to individual measurements. Following similar arguments we arrive at

$$(\boldsymbol{\beta} - \bar{\boldsymbol{\beta}})^{\mathrm{T}} s_{\bar{\boldsymbol{\beta}}}^{-1} (\boldsymbol{\beta} - \bar{\boldsymbol{\beta}}) = t_P^2(3, m-3) \tag{C.11}$$

as here the elements of the empirical variance–covariance matrix $s_{\bar{\boldsymbol{\beta}}}$ have degrees of freedom $m-3$. Hence, we have to refer to the quantiles of the density

$$p_T(t; 3, m-3)$$

$$= \frac{2\Gamma[(m-2)/2]}{(m-3)^{3/2}\Gamma[(m-5)/2]\,\Gamma(3/2)} \frac{t^2}{\left[1 + \dfrac{t^2}{m-3}\right]^{(m-2)/2}} \tag{C.12}$$

for 3 variables and $m-3$ degrees of freedom.

D Extreme Points of Ellipses and Ellipsoids

To facilitate graphical representations of ellipses and ellipsoids we draw upon their extreme points.

Confidence Ellipses

The extreme point of the confidence ellipse (13.27) with respect to the β_1- and β_2-directions are given by

$$\begin{pmatrix} \bar{\beta}_1 \\ \bar{\beta}_2 \end{pmatrix}_{\beta_1\text{-direction}} = \pm \frac{t}{\sqrt{s_{xx}}} \begin{pmatrix} s_{xx} \\ s_{xy} \end{pmatrix} \tag{D.1}$$

and

$$\begin{pmatrix} \bar{\beta}_1 \\ \bar{\beta}_2 \end{pmatrix}_{\beta_2\text{-direction}} = \pm \frac{t}{\sqrt{s_{yy}}} \begin{pmatrix} s_{yx} \\ s_{yy} \end{pmatrix} , \tag{D.2}$$

respectively. Correspondingly, for (14.26) we have

$$\begin{pmatrix} \bar{\beta}_1 \\ \bar{\beta}_2 \end{pmatrix}_{\beta_1\text{-direction}} = \pm \frac{t}{\sqrt{n}\sqrt{s_{xx}}} \begin{pmatrix} s_{xx} \\ s_{xy} \end{pmatrix} \tag{D.3}$$

and

$$\begin{pmatrix} \bar{\beta}_1 \\ \bar{\beta}_2 \end{pmatrix}_{\beta_2\text{-direction}} = \pm \frac{t}{\sqrt{n}\sqrt{s_{yy}}} \begin{pmatrix} s_{yx} \\ s_{yy} \end{pmatrix} . \tag{D.4}$$

Confidence Ellipsoids

With respect to ellipsoids, let us start out considering

$$\boldsymbol{x}^{\mathrm{T}} \boldsymbol{s}^{-\mathbf{1}} \boldsymbol{x} = t^2/n \tag{D.5}$$

where $\boldsymbol{x} = (x \quad y \quad z)^{\mathrm{T}}$ marks any point on the ellipsoid's skin. Furthermore, let

$$\boldsymbol{s} = \begin{pmatrix} s_{11} & s_{12} & s_{13} \\ s_{21} & s_{22} & s_{23} \\ s_{31} & s_{32} & s_{33} \end{pmatrix} \tag{D.6}$$

denote the empirical variance–covariance matrix and

$$\text{adj } \boldsymbol{s} = \begin{pmatrix} \rho_{11} & \rho_{21} & \rho_{31} \\ \rho_{12} & \rho_{22} & \rho_{32} \\ \rho_{13} & \rho_{23} & \rho_{33} \end{pmatrix} \tag{D.7}$$

its adjoint, with ρ_{ij} the cofactors of s_{ij}, both matrices being symmetrical. As is well known, we have

$$\boldsymbol{s}^{-1} = \frac{\text{adj } \boldsymbol{s}}{|\boldsymbol{s}\,|} \tag{D.8}$$

with $|\boldsymbol{s}\,|$ the determinant of $\boldsymbol{s}$. In the following we shall refer to the relations

$$\begin{aligned} |\boldsymbol{s}\,|s_{11} &= \rho_{22}\rho_{33} - \rho_{32}\rho_{23}\,, & |\boldsymbol{s}\,|s_{22} &= \rho_{11}\rho_{33} - \rho_{13}\rho_{31} \\ |\boldsymbol{s}\,|s_{12} &= \rho_{31}\rho_{23} - \rho_{21}\rho_{33}\,, & |\boldsymbol{s}\,|s_{23} &= \rho_{12}\rho_{31} - \rho_{11}\rho_{32} \\ |\boldsymbol{s}\,|s_{13} &= \rho_{21}\rho_{32} - \rho_{22}\rho_{13}\,, & |\boldsymbol{s}\,|s_{33} &= \rho_{11}\rho_{22} - \rho_{12}\rho_{21} \end{aligned} \tag{D.9}$$

and

$$\begin{aligned} \rho_{11}s_{31} + \rho_{21}s_{32} + \rho_{31}s_{33} &= 0 \\ \rho_{12}s_{31} + \rho_{22}s_{32} + \rho_{32}s_{33} &= 0 \\ \rho_{13}s_{31} + \rho_{23}s_{32} + \rho_{33}s_{33} &= |\boldsymbol{s}\,|\,. \end{aligned} \tag{D.10}$$

From (D.5) and (D.8) we draw

$$\begin{gathered} f(x, y, z) = \\ \rho_{11}x^2 + \rho_{22}y^2 + \rho_{33}z^2 + 2\rho_{12}xy + 2\rho_{23}yz + 2\rho_{31}zx - \frac{t^2}{n}\,|\,\boldsymbol{s}\,| = 0\,. \end{gathered} \tag{D.11}$$

Let $(x_1 \quad y_1 \quad z_1)^{\mathrm{T}}$ denote one of the two extreme points in the z-direction. The respective normal vector is given by $(0 \quad 0 \quad \partial f/\partial z)^{\mathrm{T}}$. Hence

$$\begin{aligned} \rho_{11}x_1 + \rho_{12}y_1 + \rho_{31}z_1 &= 0 \\ \rho_{12}x_1 + \rho_{22}y_1 + \rho_{23}z_1 &= 0 \\ \rho_{31}x_1 + \rho_{23}y_1 + \rho_{33}z_1 &= \frac{\partial f}{\partial z}\,. \end{aligned} \tag{D.12}$$

Solving for x_1, y_1, z_1 yields

$$\begin{aligned} x_1 &= \frac{1}{|\boldsymbol{s}|^2}\frac{\partial f}{\partial z}\,(\rho_{12}\rho_{23} - \rho_{31}\rho_{22}) = \frac{1}{|\boldsymbol{s}|}\frac{\partial f}{\partial z}\,s_{13} \\ y_1 &= \frac{1}{|\boldsymbol{s}|^2}\frac{\partial f}{\partial z}\,(\rho_{12}\rho_{31} - \rho_{23}\rho_{11}) = \frac{1}{|\boldsymbol{s}|}\frac{\partial f}{\partial z}\,s_{23} \\ z_1 &= \frac{1}{|\boldsymbol{s}|^2}\frac{\partial f}{\partial z}\,(\rho_{11}\rho_{22} - \rho_{12}\rho_{12}) = \frac{1}{|\boldsymbol{s}|}\frac{\partial f}{\partial z}\,s_{33}\,. \end{aligned} \tag{D.13}$$

Inserting this into (D.11) we find

$$\frac{\partial f}{\partial z} = \pm\frac{1}{\sqrt{s_{33}}}\,|\boldsymbol{s}|\frac{t}{\sqrt{n}}\,. \tag{D.14}$$

Analogue procedures lead to the extreme points in the x- and y-direction, respectively. Returning to the center coordinates $\bar{\beta}_1$, $\bar{\beta}_2$, and $\bar{\beta}_3$ we have

in the β_1-direction

$$\begin{pmatrix} \bar{\beta}_1 \\ \bar{\beta}_2 \\ \bar{\beta}_3 \end{pmatrix}_{\beta_1\text{-direction}} = \pm\frac{t}{\sqrt{n}\sqrt{s_{11}}}\begin{pmatrix} s_{11} \\ s_{12} \\ s_{13} \end{pmatrix}, \tag{D.15}$$

in the β_2-direction

$$\begin{pmatrix} \bar{\beta}_1 \\ \bar{\beta}_2 \\ \bar{\beta}_3 \end{pmatrix}_{\beta_2\text{-direction}} = \pm\frac{t}{\sqrt{n}\sqrt{s_{22}}}\begin{pmatrix} s_{21} \\ s_{22} \\ s_{23} \end{pmatrix} \tag{D.16}$$

and, finally, in the β_3-direction

$$\begin{pmatrix} \bar{\beta}_1 \\ \bar{\beta}_2 \\ \bar{\beta}_3 \end{pmatrix}_{\beta_3\text{-direction}} = \pm\frac{t}{\sqrt{n}\sqrt{s_{33}}}\begin{pmatrix} s_{31} \\ s_{32} \\ s_{33} \end{pmatrix}. \tag{D.17}$$

E Drawing Ellipses and Ellipsoids

Just for convenience, we summarize the basic formulas to be used to draw ellipses and ellipsoids.

Ellipses

To have an example, we refer to (13.27),

$$s_{\bar\beta_2\bar\beta_2}(\beta_1-\bar\beta_1)^2 - 2s_{\bar\beta_1\bar\beta_2}(\beta_1-\bar\beta_1)(\beta_2-\bar\beta_2) + s_{\bar\beta_1\bar\beta_1}(\beta_2-\bar\beta_2)^2$$

$$= t_P^2(2,m-2)|\boldsymbol{s}_{\bar{\boldsymbol{\beta}}}\,|\,.$$

Putting

$$\beta_1-\bar\beta_1 = r\cos\varphi; \qquad \beta_2-\bar\beta_2 = r\sin\varphi$$

we have

$$r = \frac{t_P(2,m-2)\sqrt{|\boldsymbol{s}_{\bar{\boldsymbol{\beta}}}\,|}}{\sqrt{s_{\bar\beta_2\bar\beta_2}\cos^2\varphi - 2s_{\bar\beta_1\bar\beta_2}\sin\varphi\cos\varphi + s_{\bar\beta_1\bar\beta_1}\sin^2\varphi}}\,.$$

In case of (14.26)

$$s_{\bar\beta_2\bar\beta_2}\left(\beta_1-\bar\beta_1\right)^2 - 2s_{\bar\beta_1\bar\beta_2}\left(\beta_1-\bar\beta_1\right)\left(\beta_2-\bar\beta_2\right) + s_{\bar\beta_1\bar\beta_1}\left(\beta_2-\bar\beta_2\right)^2$$

$$= |\ \boldsymbol{s}_{\bar{\boldsymbol{\beta}}}\ |\ \frac{t_P^2(2,n-1)}{n}$$

we find

$$r = \frac{\dfrac{t_P(2,n-1)}{\sqrt{n}}\ \sqrt{|\boldsymbol{s}_{\bar{\boldsymbol{\beta}}}\,|}}{\sqrt{s_{\bar\beta_2\bar\beta_2}\cos^2\varphi - 2s_{\bar\beta_1\bar\beta_2}\sin\varphi\cos\varphi + s_{\bar\beta_1\bar\beta_1}\sin^2\varphi}}\,.$$

Ellipsoids

We refer to (17.22),

$$(\boldsymbol{\beta} - \bar{\boldsymbol{\beta}})^{\mathrm{T}} s_{\bar{\boldsymbol{\beta}}}^{-1} (\boldsymbol{\beta} - \bar{\boldsymbol{\beta}}) = t_P^2(3, m-3)\,, \tag{E.1}$$

with $s_{\bar{\boldsymbol{\beta}}}$ as given in (17.14),

$$\boldsymbol{s}_{\bar{\beta}} = \begin{pmatrix} s_{\bar{\beta}_1\bar{\beta}_1} & s_{\bar{\beta}_1\bar{\beta}_2} & s_{\bar{\beta}_1\bar{\beta}_3} \\ s_{\bar{\beta}_2\bar{\beta}_1} & s_{\bar{\beta}_2\bar{\beta}_2} & s_{\bar{\beta}_2\bar{\beta}_3} \\ s_{\bar{\beta}_3\bar{\beta}_1} & s_{\bar{\beta}_3\bar{\beta}_2} & s_{\bar{\beta}_3\bar{\beta}_3} \end{pmatrix}.$$

To shorten the notation we put

$$x = \beta_1 - \bar{\beta}_1\,, \qquad y = \beta_2 - \bar{\beta}_2\,, \qquad z = \beta_3 - \bar{\beta}_3$$

and, in a formal sense,

$$s_{\bar{\boldsymbol{\beta}}}^{-1} = \begin{pmatrix} \gamma_{11} & \gamma_{12} & \gamma_{13} \\ \gamma_{21} & \gamma_{22} & \gamma_{23} \\ \gamma_{31} & \gamma_{32} & \gamma_{33} \end{pmatrix} \tag{E.2}$$

so that (E.1) turns into

$$\gamma_{11}x^2 + \gamma_{22}y^2 + \gamma_{33}z^2 + 2\gamma_{12}xy + 2\gamma_{23}yz + 2\gamma_{31}zx = t_P^2(3, m-2)\,. \tag{E.3}$$

The contour lines $z =$ const. are obviously ellipses. Following (D.17), we have to consider the interval

$$-\,t_P(3, m-3)\sqrt{s_{\bar{\beta}_3\bar{\beta}_3}} \le z \le t_P(3, m-3)\sqrt{s_{\bar{\beta}_3\bar{\beta}_3}}\,. \tag{E.4}$$

As the centers of the ellipses are shifted with respect to the origin $x = y = 0$, we put

$$x = \xi + x_M; \qquad y = \eta + y_M \tag{E.5}$$

where

$$x_M = \frac{\gamma_{22}\gamma_{31} - \gamma_{12}\gamma_{23}}{\gamma_{12}^2 - \gamma_{11}\gamma_{22}}\, z\,; \qquad y_M = \frac{\gamma_{11}\gamma_{23} - \gamma_{12}\gamma_{31}}{\gamma_{12}^2 - \gamma_{11}\gamma_{22}}\, z\,. \tag{E.6}$$

For any z=const. we have

$$\begin{aligned} \gamma_{11}\xi^2 + 2\gamma_{12}\xi\eta + \gamma_{22}\eta^2 &= t_P^2(3, m-3) \\ -(\gamma_{33}z^2 + 2(\gamma_{31}x_M + \gamma_{23}y_M)z &+ \gamma_{11}x_M^2 + 2\gamma_{12}x_M\,y_M + \gamma_{22}y_M^2)\,. \end{aligned} \tag{E.7}$$

After all, the problem to draw a spatially rotated ellipsoid has been reduced to the problem to draw a sufficiently dense set of ellipses perpendicular to the z-axis.

F Security Polygons and Polyhedra

Unknown systematic errors cause a new, in error calculus hitherto unknown species of geometrical objects to go on stage [8]. These are polygons in case of two measurands, polyhedra in case of three and abstract polytopes for more than three measurands. At any rate, the objects are convex and point-symmetric [28]. The naming security polygon, security polyhedron and security polytope establishes a correspondence to the terms confidence ellipse and confidence ellipsoid. We shall confine ourselves to polygons and polyhedra.

Security Polygons

Edges

Let us reconsider (14.10). For $r = 2$ the components of the propagated systematic error

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

span a polygon. In a way, the polygon comes into being while the $f_{\bar{y}_1}, f_{\bar{y}_1}, \ldots,$ $f_{\bar{y}_m}$ "scan" the set of points lying within or on the faces of the m-dimensional hypercuboid

$$-f_{s,\bar{y}_i} \le f_{\bar{y}_i} \le f_{s,\bar{y}_i} ; \quad i = 1, \ldots, m\,.$$

To simplify matters, let us put $f_{\bar{y}_i} = f_i,\ f_{s,\bar{y}_i} = f_{s,i}$ and $m = 5$ so that

$$\begin{aligned} f_{\bar{\beta}_1} &= b_{11} f_1 + b_{21} f_2 + b_{31} f_3 + b_{41} f_4 + b_{51} f_5 \\ f_{\bar{\beta}_2} &= b_{12} f_1 + b_{22} f_2 + b_{32} f_3 + b_{42} f_4 + b_{52} f_5 \end{aligned} \qquad \text{(F.1)}$$

with

$$- f_{s,i} \le f_i \le f_{s,i} ; \quad i = 1, \ldots, 5\,. \qquad \text{(F.2)}$$

With reference to a rectangular $f_{\bar{\beta}_1}, f_{\bar{\beta}_2}$ coordinate system, the polygon is obviously enclosed within a rectangle

$$-f_{s,\bar{\beta}_k} \le f_{\bar{\beta}_k} \le f_{s,\bar{\beta}_k}\,; \quad f_{s,\bar{\beta}_k} = \sum_{i=1}^{5} |b_{ik}|\, f_{s,i}\,; \quad k = 1,2\,.$$

Let us assume $b_{11} \neq 0$. Eliminating f_1, we find a straight line

$$f_{\bar{\beta}_2} = \frac{b_{12}}{b_{11}} f_{\bar{\beta}_1} + c_1 \tag{F.3}$$

where

$$c_1 = h_{12} f_2 + h_{13} f_3 + h_{14} f_4 + h_{15} f_5$$

and

$$h_{12} = \frac{1}{b_{11}} (b_{11} b_{22} - b_{12} b_{21})\,, \qquad h_{13} = \frac{1}{b_{11}} (b_{11} b_{32} - b_{12} b_{31})$$

$$h_{14} = \frac{1}{b_{11}} (b_{11} b_{42} - b_{12} b_{41})\,, \qquad h_{15} = \frac{1}{b_{11}} (b_{11} b_{52} - b_{12} b_{51})\,.$$

Any variation of c_1 shifts the line (F.3) parallel to itself; c_1 is maximal if

$$\begin{aligned} f_2 &= f_2^* = \operatorname{sign}(h_{12})\, f_{s,2}\,, \quad f_3 = f_3^* = \operatorname{sign}(h_{13})\, f_{s,3} \\ f_4 &= f_4^* = \operatorname{sign}(h_{14})\, f_{s,4}\,, \quad f_5 = f_5^* = \operatorname{sign}(h_{15})\, f_{s,5}\,. \end{aligned} \tag{F.4}$$

We obviously have

$$c_{s,1} = h_{12} f_2^* + h_{13} f_3^* + h_{14} f_4^* + h_{15} f_5^*$$

and

$$-\,c_{s,1} \le c_1 \le c_{s,1}\,. \tag{F.5}$$

Hence, the lines

$$f_{\bar{\beta}_2} = \frac{b_{12}}{b_{11}} f_{\bar{\beta}_1} + c_{s,1}\,, \qquad f_{\bar{\beta}_2} = \frac{b_{12}}{b_{11}} f_{\bar{\beta}_1} - c_{s,1} \tag{F.6}$$

hold maximum distance thus pegging two edges of the polygon. Shifting f_1 in $-f_{s,1},\ \ldots,\ f_{s,1}$, the point

$$\begin{aligned} f_{\bar{\beta}_1} &= b_{11} f_1 + b_{21} f_2^* + b_{31} f_3^* + b_{41} f_4^* + b_{51} f_5^* \\ f_{\bar{\beta}_2} &= b_{12} f_1 + b_{22} f_2^* + b_{32} f_3^* + b_{42} f_4^* + b_{52} f_5^*\,, \end{aligned} \tag{F.7}$$

slides along the polygon's $c_{s,1}$ edge and something similar applies to the $-c_{s,1}$ edge.

Vertices

When it comes to specify the vertices of the two edges obtained so far, the $c_{s,1}$ edge is marked off by

$$\text{Vertex} \quad V_1$$

$$f_{\bar{\beta}_1,1} = b_{11} f_{s,1} + b_{21} f_2^* + b_{31} f_3^* + b_{41} f_4^* + b_{51} f_5^*$$

$$f_{\bar{\beta}_2,1} = b_{12} f_{s,1} + b_{22} f_2^* + b_{32} f_3^* + b_{42} f_4^* + b_{52} f_5^*$$

and

$$\text{Vertex} \quad V_2$$

$$f_{\bar{\beta}_1,2} = -b_{11} f_{s,1} + b_{21} f_2^* + b_{31} f_3^* + b_{41} f_4^* + b_{51} f_5^*$$

$$f_{\bar{\beta}_2,2} = -b_{12} f_{s,1} + b_{22} f_2^* + b_{32} f_3^* + b_{42} f_4^* + b_{52} f_5^* \,.$$

For the $-c_{s,1}$ edge we have

$$\text{Vertex} \quad V_3$$

$$f_{\bar{\beta}_1,3} = b_{11} f_{s,1} - b_{21} f_2^* - b_{31} f_3^* - b_{41} f_4^* - b_{51} f_5^*$$

$$f_{\bar{\beta}_2,3} = b_{12} f_{s,1} - b_{22} f_2^* - b_{32} f_3^* - b_{42} f_4^* - b_{52} f_5^*$$

and

$$\text{Vertex} \quad V_4$$

$$f_{\bar{\beta}_1,4} = -b_{11} f_{s,1} - b_{21} f_2^* - b_{31} f_3^* - b_{41} f_4^* - b_{51} f_5^*$$

$$f_{\bar{\beta}_2,4} = -b_{12} f_{s,1} - b_{22} f_2^* - b_{32} f_3^* - b_{42} f_4^* - b_{52} f_5^* \,.$$

This suggests a point symmetry with respect to the vertices V_1 and V_4 and the vertices V_2 and V_3, respectively. After all, we have found two of the polygon's edges including their vertices. We conclude that the polygon holds at most m pairs of parallel edges.

Given $b_{11} = 0$, we cannot eliminate f_1. Instead, (F.1) produces two abscissas

$$\begin{aligned} f_{\bar{\beta}_1} = \pm \quad & [\operatorname{sign}(b_{21})\, b_{21} f_{s,2} + \operatorname{sign}(b_{31})\, b_{31} f_{s,3} \\ & + \operatorname{sign}(b_{41})\, b_{41} f_{s,4} + \operatorname{sign}(b_{51})\, b_{51} f_{s,5} \,] \end{aligned} \tag{F.8}$$

through each of which a line is to be drawn parallel to the $f_{\bar{\beta}_2}$-axis. The coordinate $f_{\bar{\beta}_2}$ slides along these verticals following

$$\begin{aligned} f_{\bar{\beta}_2} = b_{12} f_1 \pm \; & [\operatorname{sign}(b_{21})\, b_{22} f_{s,2} + \operatorname{sign}(b_{31})\, b_{32} f_{s,3} \\ & + \quad \operatorname{sign}(b_{41})\, b_{42} f_{s,4} + \operatorname{sign}(b_{51})\, b_{52} f_{s,5} \,] \,. \end{aligned} \tag{F.9}$$

Equal systematic errors

Assuming $f_{\bar{y}_i} = f_y\,;\; f_{s,\bar{y}_i} = f_{s,y};\;\; i = 1,\,\ldots\,,m$, due to (14.13), the security polygon degenerates into an interval

$$-\,f_{s,y} \le f_{s,\bar{\beta}_1} \le f_{s,y}\,; \qquad f_{\bar{\beta}_2} = 0\,. \tag{F.10}$$

Security Polyhedra

Faces

To examine the geometrical properties of the convex, point-symmetric hull spanned by three propagated systematic errors,

$$f_{\bar{\beta}_k} = \sum_{i=1}^{m} b_{ik} f_i\,, \quad -f_{s,i} \le f_i \le f_{s,i}\,; \qquad k = 1,2,3$$

we again confine ourselves to $m = 5$

$$\begin{aligned} f_{\bar{\beta}_1} &= b_{11}f_1 + b_{21}f_2 + b_{31}f_3 + b_{41}f_4 + b_{51}f_5 \\ f_{\bar{\beta}_2} &= b_{12}f_1 + b_{22}f_2 + b_{32}f_3 + b_{42}f_4 + b_{52}f_5 \\ f_{\bar{\beta}_3} &= b_{13}f_1 + b_{23}f_2 + b_{33}f_3 + b_{43}f_4 + b_{53}f_5\,. \end{aligned} \tag{F.11}$$

With respect to a rectangular $f_{\bar{\beta}_1}, f_{\bar{\beta}_2}, f_{\bar{\beta}_3}$ coordinate system, the polyhedron is enclosed within a cuboid given by

$$-\,f_{s,\bar{\beta}_k} \le f_{\bar{\beta}_k} \le f_{s,\bar{\beta}_k}\,; \quad f_{s,\bar{\beta}_k} = \sum_{i=1}^{5} |b_{ik}|\, f_{s,i}\,; \quad k = 1,2,3\,. \tag{F.12}$$

Rewriting (F.11) according to

$$\begin{aligned} b_{11}f_1 + b_{21}f_2 + b_{31}f_3 &= f_{\bar{\beta}_1} - b_{41}f_4 - b_{51}f_5 = \xi \\ b_{12}f_1 + b_{22}f_2 + b_{32}f_3 &= f_{\bar{\beta}_2} - b_{42}f_4 - b_{52}f_5 = \eta \\ b_{13}f_1 + b_{23}f_2 + b_{33}f_3 &= f_{\bar{\beta}_3} - b_{43}f_4 - b_{53}f_5 = \zeta \end{aligned} \tag{F.13}$$

we may eliminate f_1 and f_2 thus solving for f_3

$$f_3 \begin{vmatrix} b_{11} & b_{21} & b_{31} \\ b_{12} & b_{22} & b_{32} \\ b_{13} & b_{23} & b_{33} \end{vmatrix} = \begin{vmatrix} b_{11} & b_{21} & \xi \\ b_{12} & b_{22} & \eta \\ b_{13} & b_{23} & \zeta \end{vmatrix}\,.$$

Defining

$$\lambda_{12} = b_{12}b_{23} - b_{22}b_{13}\,, \quad \mu_{12} = b_{21}b_{13} - b_{11}b_{23}\,, \quad \nu_{12} = b_{11}b_{22} - b_{21}b_{12}$$

we have

$$\lambda_{12} f_{\bar{\beta}_1} + \mu_{12} f_{\bar{\beta}_2} + \nu_{12} f_{\bar{\beta}_3} = c_{12} \tag{F.14}$$

where

$$c_{12} = h_{12,3} f_3 + h_{12,4} f_4 + h_{12,5} f_5 \tag{F.15}$$

and

$$\begin{aligned} h_{12,3} &= (\lambda_{12} b_{31} + \mu_{12} b_{32} + \nu_{12} b_{33}) \\ h_{12,4} &= (\lambda_{12} b_{41} + \mu_{12} b_{42} + \nu_{12} b_{43}) \\ h_{12,5} &= (\lambda_{12} b_{51} + \mu_{12} b_{52} + \nu_{12} b_{53}) \,. \end{aligned}$$

Varying c_{12}, which we can do via f_3, f_4, f_5, the plane (F.14) gets shifted parallel to itself. The choices

$$\begin{aligned} f_3 &= f_3^* = \operatorname{sign}(h_{12,3})\, f_{s,3} \\ f_4 &= f_4^* = \operatorname{sign}(h_{12,4})\, f_{s,4} \\ f_5 &= f_5^* = \operatorname{sign}(h_{12,5})\, f_{s,5} \end{aligned}$$

assign a maximum value to c_{12}

$$c_{s,12} = h_{12,3} f_3^* + h_{12,4} f_4^* + h_{12,5} f_5^*$$

whereat

$$-c_{s,12} \le c_{12} \le c_{s,12} \,.$$

After all, we have found two of the solid's faces. Calling them F1 and F2, we observe

$$\begin{aligned} \lambda_{12} f_{\bar{\beta}_1} + \mu_{12} f_{\bar{\beta}_2} + \nu_{12} f_{\bar{\beta}_3} &= -c_{s,12} \qquad \text{F1} \\ \lambda_{12} f_{\bar{\beta}_1} + \mu_{12} f_{\bar{\beta}_2} + \nu_{12} f_{\bar{\beta}_3} &= c_{s,12} \qquad \text{F2}\,. \end{aligned} \tag{F.16}$$

In

$$\boldsymbol{f} = (f_1 \quad f_2 \quad f_3 \quad f_4 \quad f_5)^{\mathrm{T}}$$

the variables f_1, f_2 are free to vary, while the variables f_3, f_4, f_5 are to be kept fixed. If f_1, f_2 vary, the vector $\boldsymbol{f}_{\bar{\boldsymbol{\beta}}} = \boldsymbol{B}^{\mathrm{T}} \boldsymbol{f}$ slides along the faces F1 and F2. Cyclically swapping the variables, we successively find the polyhedron's remaining faces. As Table F.1 indicates, the maximum number of faces is given by $m(m-1)$. Table F.2 visualizes the swapping procedure.

Given in (F.11), say, b_{11} and b_{12} vanish, we cannot eliminate f_1. Moreover, as ν_{12} becomes zero, (F.16) represents a pair of planes parallel to the $f_{\bar{\beta}_3}$-axis,

$$\lambda_{12} f_{\bar{\beta}_1} + \mu_{12} f_{\bar{\beta}_2} = \pm c_{s,12}\,; \quad \nu_{12} = 0\,.$$

The cases $\lambda_{12} = 0$ and $\mu_{12} = 0$ are to be treated correspondingly.

Table F.1. Maximum Number of Faces

×	$f_1 f_2$	$f_1 f_3$	$f_1 f_4$	$f_1 f_5$
×	×	$f_2 f_3$	$f_2 f_4$	$f_2 f_5$
×	×	×	$f_3 f_4$	$f_3 f_5$
×	×	×	×	$f_4 f_5$
×	×	×	×	×

Table F.2. Cyclic Elimination, $r = 3$ and $m = 5$

	Eliminated variable			Variables remaining within the system		
1st step	f_1	f_2	$\Rightarrow$	f_3	f_4	f_5
2nd step	f_1	f_3	$\Rightarrow$	f_4	f_5	f_2
3rd step	f_1	f_4	$\Rightarrow$	f_5	f_2	f_3
4th step	f_1	f_5	$\Rightarrow$	f_2	f_3	f_4
5th step	f_2	f_3	$\Rightarrow$	f_4	f_5	f_1
6th step	f_2	f_4	$\Rightarrow$	f_5	f_1	f_3
7th step	f_2	f_5	$\Rightarrow$	f_1	f_3	f_4
8th step	f_3	f_4	$\Rightarrow$	f_5	f_1	f_2
9th step	f_3	f_5	$\Rightarrow$	f_1	f_2	f_4
10th step	f_4	f_5	$\Rightarrow$	f_1	f_2	f_3

Vertices

Given $h_{12,i} \neq 0$; $i = 3, 4, 5$, we may consider two sets of $\boldsymbol{f}$-vectors with respect to the faces F1 and F2, namely

$$\begin{array}{l} [\,-f_{s,1} \quad -f_{s,2} \quad -f_3^* \quad -f_4^* \quad -f_5^*\,]^{\mathrm{T}} \\ [\,f_{s,1} \quad -f_{s,2} \quad -f_3^* \quad -f_4^* \quad -f_5^*\,]^{\mathrm{T}} \\ [\,-f_{s,1} \quad f_{s,2} \quad -f_3^* \quad -f_4^* \quad -f_5^*\,]^{\mathrm{T}} \\ [\,f_{s,1} \quad f_{s,2} \quad -f_3^* \quad -f_4^* \quad -f_5^*\,]^{\mathrm{T}} \end{array} \qquad \text{F1}$$

and

$$\begin{array}{l} [\,f_{s,1} \quad f_{s,2} \quad f_3^* \quad f_4^* \quad f_5^*\,]^{\mathrm{T}} \\ [\,-f_{s,1} \quad f_{s,2} \quad f_3^* \quad f_4^* \quad f_5^*\,]^{\mathrm{T}} \\ [\,f_{s,1} \quad -f_{s,2} \quad f_3^* \quad f_4^* \quad f_5^*\,]^{\mathrm{T}} \\ [\,-f_{s,1} \quad -f_{s,2} \quad f_3^* \quad f_4^* \quad f_5^*\,]^{\mathrm{T}} \end{array} \qquad \text{F2}$$

On each of the faces, these vectors appoint four vertices via $\boldsymbol{f}_{\bar{\boldsymbol{\beta}}} = \boldsymbol{B}^{\mathrm{T}}\boldsymbol{f}$. For F1, we find

Vertex V_1

$$f_{\bar{\beta}_1,1} = -b_{11}f_{s,1} - b_{21}f_{s,2} - b_{31}f_3^* - b_{41}f_4^* - b_{51}f_5^*$$

$$f_{\bar{\beta}_2,1} = -b_{12}f_{s,1} - b_{22}f_{s,2} - b_{32}f_3^* - b_{42}f_4^* - b_{52}f_5^*$$

$$f_{\bar{\beta}_3,1} = -b_{13}f_{s,1} - b_{23}f_2 - b_{33}f_3^* - b_{43}f_4^* - b_{52}f_5^*$$

Vertex V_2

$$f_{\bar{\beta}_1,1} = b_{11}f_{s,1} - b_{21}f_{s,2} - b_{31}f_3^* - b_{41}f_4^* - b_{51}f_5^*$$

$$f_{\bar{\beta}_2,1} = b_{12}f_{s,1} - b_{22}f_{s,2} - b_{32}f_3^* - b_{42}f_4^* - b_{52}f_5^*$$

$$f_{\bar{\beta}_3,1} = b_{13}f_{s,1} - b_{23}f_{s,2} - b_{33}f_3^* - b_{43}f_4^* - b_{52}f_5^*$$

Vertex V_3

$$f_{\bar{\beta}_1,1} = -b_{11}f_{s,1} + b_{21}f_{s,2} - b_{31}f_3^* - b_{41}f_4^* - b_{51}f_5^*$$

$$f_{\bar{\beta}_2,1} = -b_{12}f_{s,1} + b_{22}f_{s,2} - b_{32}f_3^* - b_{42}f_4^* - b_{52}f_5^*$$

$$f_{\bar{\beta}_3,1} = -b_{13}f_{s,1} + b_{23}f_{s,2} - b_{33}f_3^* - b_{43}f_4^* - b_{52}f_5^*$$

Vertex V_4

$$f_{\bar{\beta}_1,1} = b_{11}f_{s,1} + b_{21}f_{s,2} - b_{31}f_3^* - b_{41}f_4^* - b_{51}f_5^*$$

$$f_{\bar{\beta}_2,1} = b_{12}f_{s,1} + b_{22}f_{s,2} - b_{32}f_3^* - b_{42}f_4^* - b_{52}f_5^*$$

$$f_{\bar{\beta}_3,1} = b_{13}f_{s,1} + b_{23}f_{s,2} - b_{33}f_3^* - b_{43}f_4^* - b_{52}f_5^*$$

As the polyhedra are point-symmetric, the vertices on F2 are to be obtained from those on F1 by mirroring.

Now assume $h_{12,5}$ to vanish. Then, as (F.11) and (F.15) suggest, each of the faces carries eight vertices instead of four. Should additionally $h_{12,4}$ vanish, each face would hold 16 vertices. However, at least one of the coefficients $h_{12,i}$, $i = 3, 4, 5$ must be unequal to zero as otherwise the planes F1 and F2 would pass through the origin.

Example

We shall find the surfaces and vertices of the polyhedron

$$\boldsymbol{f}_{\bar{\beta}} = \boldsymbol{B}^{\mathrm{T}} \boldsymbol{f} \,, \quad \boldsymbol{B}^{\mathrm{T}} = \begin{pmatrix} 1 & 2 & 3 & -1 & 2 \\ -1 & 3 & 2 & 2 & -1 \\ 2 & -1 & -3 & 3 & -3 \end{pmatrix} , \quad -1 \le f_i \le 1 \,; \quad i = 1, \ldots, 4 \,.$$

As suggested by

$$\begin{aligned} f_{\bar{\beta}_1} &= f_1 + 2f_2 + 3f_3 - f_4 + 2f_5 \\ f_{\bar{\beta}_2} &= -f_1 + 3f_2 + 2f_3 + 2f_4 - f_5 \\ f_{\bar{\beta}_3} &= 2f_1 - f_2 - 3f_3 + 3f_4 - 3f_5 \,, \end{aligned}$$

the polyhedron is enclosed within the cuboid

$$-9 \le f_{\bar{\beta}_1} \le 9 \,, \quad -9 \le f_{\bar{\beta}_2} \le 9 \,, \quad -12 \le f_{\bar{\beta}_3} \le 12 \,.$$

Cyclic elimination yields the coefficients λ, μ, ν, the constants $h_{12,3}, \ldots$ and $\pm c_{s,12}, \ldots$ and finally the vertices and faces. The polyhedron is depicted in Fig. F.1 and shows 20 faces, each face holding four vertices.

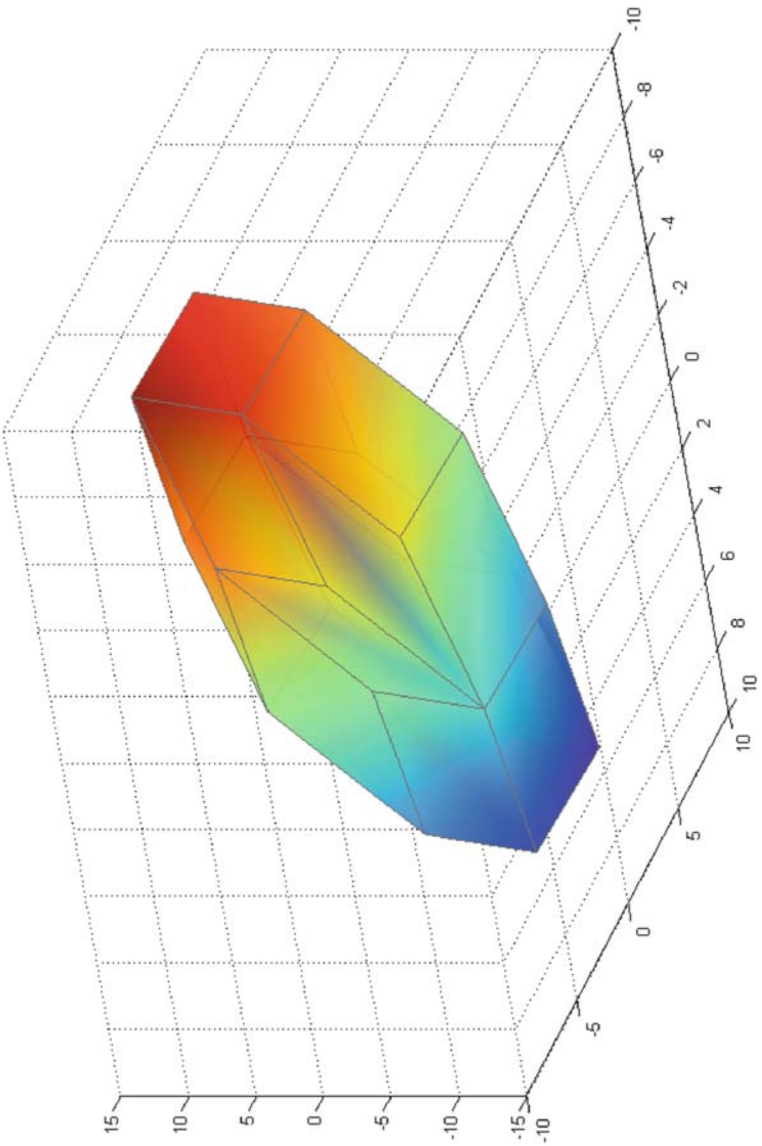

Fig. F.1. Security polyhedron as specified in the example: there are 20 faces, each face having four vertices

G EP Boundaries and EPC Hulls

The configuration of confidence ellipses and ellipsoids on the one hand with security polygons and polyhedra on the other gives rise to EP boundaries and EPC hulls as termed by the author. An EP boundary is intended to localize a 2-tuple of true values with respect to the related 2-tuple of estimators. An EPC hull does, mutatis mutandis, the same for a 3-tuple. We shall abstain from considering tuples with dimensionality greater than 3. To recall [8, 29, 28]:

- An EP boundary denotes a convex, continuously differentiable closed line composed of the segments of a confidence Ellipse and the edges of a Polygon.
- An EPC hull devises a convex, continuously differentiable closed surface composed of the segments of a confidence Ellipsoid, the faces of a Polyhedron and certain segments of elliptical Cylinders providing smooth transitions between the flat and elliptically curved parts of the hull.

While an EP boundary resembles a convex slice of a potato, an EPC hull takes after a convex potato as a whole.

EP Boundary

Ellipse and Interval

Let us consider a rectangular β_1, β_2 coordinate system and estimators $\bar{\beta}_1$, $\bar{\beta}_2$ with expectations $\mu_{\bar{\beta}_1}$, $\mu_{\bar{\beta}_2}$ and true values $\beta_{0,1}$, $\beta_{0,2}$, respectively. Any point of the ellipse's circumference may coincide with the point

$$\boldsymbol{\mu}_{\bar{\boldsymbol{\beta}}} = \begin{pmatrix} \mu_{\bar{\beta}_1} \\ \mu_{\bar{\beta}_2} \end{pmatrix} .$$

Let the interval limiting the propagated systematic error be stretched along the β_1- axes and notionally be taken as a "stick."

To span the EP region, we move the midpoint of the "stick" along the circumference of the ellipse, keeping the stick's orientation steadily horizontal, i.e. parallel to the β_1-axis. The end of the stick pointing away from the ellipse produces a point of the EP boundary. For a practical approach, we observe that there are two points of the ellipse in which the "stick" coincides with the local tangent. Here, we decompose the ellipse shifting one of the partial arcs to the left and the other to right, in each case parallel to the β_1-axis. Reconnecting the arcs on either side by copies of the horizontally kept "stick" produces the EP boundary as a whole.

We expect the tuple $(\beta_{0,1},\ \beta_{0,2})$ of true values to be an element of the set of $(\beta_1,\ \beta_2)$-tuples lying within or on the borderline of the EP region.

Ellipse and Polygon

Again, we refer to a rectangular β_1, β_2 coordinate system and estimators $\bar{\beta}_1$, $\bar{\beta}_2$ with expectations $\mu_{\bar{\beta}_1}$, $\mu_{\bar{\beta}_2}$ and true values $\beta_{0,1}$, $\beta_{0,2}$, respectively. Any point of the ellipse's circumference may coincide with the point

$$\boldsymbol{\mu}_{\bar{\boldsymbol{\beta}}} = \begin{pmatrix} \mu_{\bar{\beta}_1} \\ \mu_{\bar{\beta}_2} \end{pmatrix} .$$

Let us now move the center of the polygon in discrete, sufficiently narrow steps along the circumference of the ellipse, keeping the polygon's orientation steadily constant. In each of the breakpoints we draw a tangent to the ellipse. Shifting the tangent away from its osculation point, parallel to itself and to the ellipse's outside, it either strikes a vertex of the polygon or coincides with one of its edges at any rate marking the largest possible distance from the osculation point. In the first case we produce a point, in the latter a line segment of the EP boundary. After all, the boundary of the EP region consists of the segments of a contiguous decomposition of the ellipse's circumference and the edges of the polygon, where arcs and edges follow in succession [29].

We expect the tuple $(\beta_{0,1},\ \beta_{0,2})$ of true values to be an element of the set of $(\beta_1,\ \beta_2)$-tuples lying within or on the borderline of the EP region.

EPC Hull

Ellipsoid and Interval

We refer to a rectangular β_1, β_2, β_3 coordinate system and estimators $\bar{\beta}_1$, $\bar{\beta}_2$, $\bar{\beta}_3$ with expectations $\mu_{\bar{\beta}_1}$, $\mu_{\bar{\beta}_2}$, $\mu_{\bar{\beta}_3}$ and true values $\beta_{0,1}$, $\beta_{0,2}$, $\beta_{0,3}$, respectively. Any point of the ellipsoid's skin may coincide with the point

$$\boldsymbol{\mu}_{\bar{\boldsymbol{\beta}}} = \begin{pmatrix} \mu_{\bar{\beta}_1} \\ \mu_{\bar{\beta}_2} \\ \mu_{\bar{\beta}_3} \end{pmatrix} .$$

Let the interval limiting the propagated systematic error be stretched along the β_1-axis and notionally taken as a "stick."

For convenience, we cover the ellipsoid by an ensemble of sufficiently dense contour lines $\beta_3 = \text{const.}$ being on their part ellipses, obviously. We then move the center of the "stick" along any one of these ellipses—keeping the stick's spatial orientation steadily horizontal and parallel to the $\bar{\beta}_1$-axis. Again, there are two points in which the "stick" coincides with the local tangent. Here, we decompose the ellipse shifting one of the partial arcs to the left and the other to the right, respectively, in each case parallel to the β_1-axis. Reconnecting the arcs on either side by inserting copies of the "stick" produces a first continuous and differentiable contour line of the EPC hull. Repeating the procedure with the ellipsoid's other contour lines eventually yields the EPC hull as a whole.

We expect the triple $(\beta_{0,1}, \beta_{0,2}, \beta_{0,3})$ of true values to be an element of the set of $(\beta_1, \beta_2, \beta_3)$-tuples lying within or on the border of the EPC hull.

Ellipsoid and Polygon

We conceive a rectangular β_1, β_2, β_3 coordinate system and estimators $\bar{\beta}_1$, $\bar{\beta}_2$, $\bar{\beta}_3$ with expectations $\mu_{\bar{\beta}_1}$, $\mu_{\bar{\beta}_2}$, $\mu_{\bar{\beta}_3}$ and true values $\beta_{0,1}$, $\beta_{0,2}$, $\beta_{0,3}$, respectively. Any point of the ellipsoid's skin may coincide with the point

$$\boldsymbol{\mu}_{\bar{\boldsymbol{\beta}}} = \begin{pmatrix} \mu_{\bar{\beta}_1} \\ \mu_{\bar{\beta}_2} \\ \mu_{\bar{\beta}_3} \end{pmatrix} .$$

Let $f_{\bar{\beta}_3} = 0$ so that the polygon confining the pair $(f_{\bar{\beta}_1}, f_{\bar{\beta}_2})$ of propagated systematic error is aligned parallel to β_1, β_2-plane.

Again, we cover the ellipsoid by an ensemble of contour lines $\beta_3 = \text{const.}$ We then move the center of the polygon in discrete, sufficiently narrow steps along any such contour line $\beta_3 = \text{const.}$, keeping the polygon's orientation steadily constant and parallel to the β_1, β_2-plane. In each of the breakpoints we conceive a local tangent. Shifting the tangent away from its osculation point, parallel to itself and to the ellipse's outside, it either strikes a vertex of the polygon or coincides with one of its edges, at any rate marking the largest possible distance from the osculation point. In the first case we get a single point, in the latter a line segment of a contour line of the EPC hull. Repeating the procedure with the other contour lines of the ellipsoid successively produces the EPC hull in its entirety.

We expect the triple $(\beta_{0,1}, \beta_{0,2}, \beta_{0,3})$ of true values to be an element of the set of $(\beta_1, \beta_2, \beta_3)$-tuples lying within or on the border of the EPC hull.

Ellipsoid and Polyhedron

We refer to a rectangular β_1, β_2, β_3 coordinate system and estimators $\bar{\beta}_1$, $\bar{\beta}_2$, $\bar{\beta}_3$ with expectations $\mu_{\bar{\beta}_1}$, $\mu_{\bar{\beta}_2}$, $\mu_{\bar{\beta}_3}$ and true values $\beta_{0,1}$, $\beta_{0,2}$, $\beta_{0,3}$, respectively. Any point of the ellipsoid's skin may coincide with the point

$$\boldsymbol{\mu}_{\bar{\boldsymbol{\beta}}} = \begin{pmatrix} \mu_{\bar{\beta}_1} \\ \mu_{\bar{\beta}_2} \\ \mu_{\bar{\beta}_3} \end{pmatrix} .$$

To span the EPC hull, we move the center of the polyhedron along any contour line $\beta_3 = \text{const.}$ of the ellipsoid, keeping the spatial orientation of the polyhedron steadily constant. In each of the breakpoints we conceive a local tangent plane. We shift the plane away from its osculation point, parallel to itself and to the ellipsoid's outside so that, finally, it strikes either a vertex of the polyhedron or coincides with one of the polyhedron's edges or faces. In the first case we get a point, in the second a line segment and in the third a plane segment of the EPC hull. Repeating the procedure with the ellipsoid's other contour lines eventually produces the EPC hull as a whole (Fig. G.1).

We expect the triple $(\beta_{0,1}, \beta_{0,2}, \beta_{0,3})$ of true values to be an element of the set of $(\beta_1, \beta_2, \beta_3)$-tuples lying within or on the border of the EPC hull.

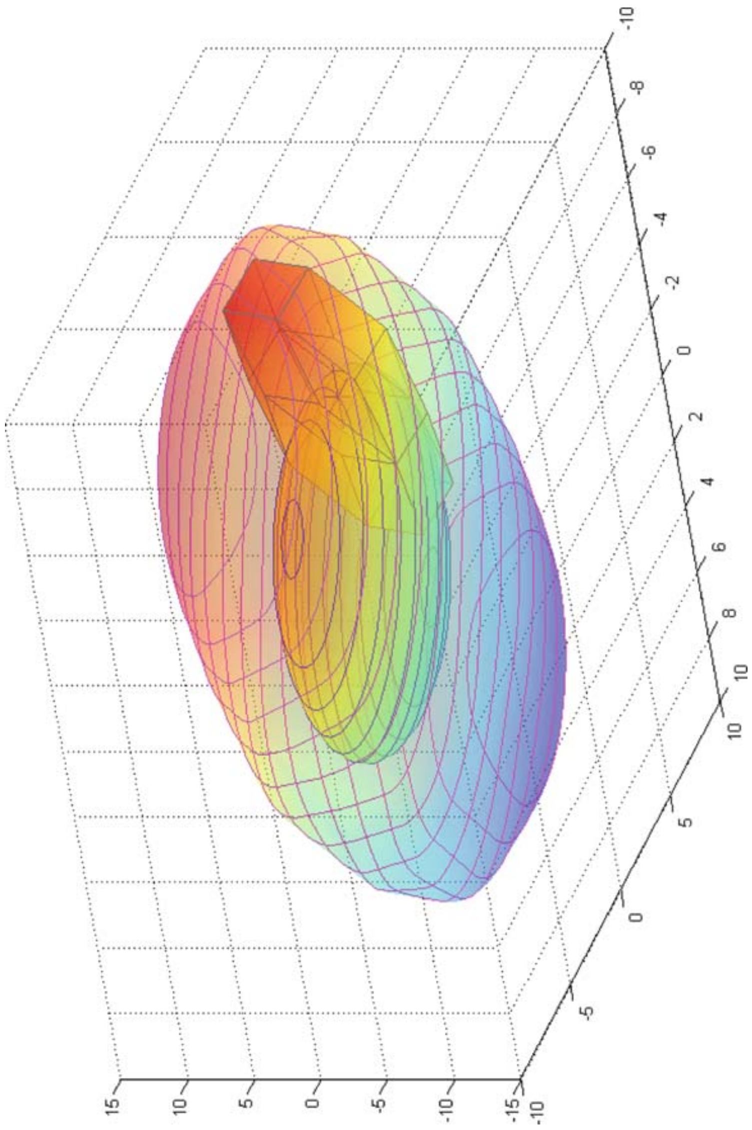

Fig. G.1. Exemplary configuration of an ellipsoid with a polyhedron

H Student's Density

We consider it beneficial to conceptualize two versions of the variable of Student's density.

Variable $\boldsymbol{T(\nu)} = \dfrac{\boldsymbol{X-\mu}}{\boldsymbol{S}}$

Let the random variable X be $N(\mu, \sigma^2)$-distributed,

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

Furthermore, let the

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

be n realization of the random variable X. The sample variance is given by

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

For a fixed t we define

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

and ask for

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

Substituting $\eta = (x-\mu)/\sigma$ for x produces

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

For this to become statistically representative, we average[1] by means of

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

so that

$$P\left(t,\nu\right) = E\left\{P\left(t,s,\nu\right)\right\} = \int\limits_{0}^{\infty} \left\{ \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{ts/\sigma} \mathrm{e}^{-\eta^2/2} \mathrm{d}\eta \right\} p_{S^2}\left(s^2\right) \mathrm{d}s^2 \,. \tag{H.8}$$

But this is a distribution function with a variable t. Hence, differentiating with respect to t

$$\frac{\mathrm{d}P\left(t,\nu\right)}{\mathrm{d}t} = \int\limits_{0}^{\infty} \left\{ \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{t^2 s^2}{2\sigma^2}\right) s \right\} p_{S^2}\left(s^2\right) \mathrm{d}s^2 \tag{H.9}$$

and integrating out the right-hand side issues a density, namely

$$p_T\left(t,\nu\right) = \frac{\Gamma\left(\dfrac{\nu+1}{2}\right)}{\sqrt{\pi\nu}\;\Gamma\left(\dfrac{\nu}{2}\right)} \frac{1}{\left(1+\dfrac{t^2}{\nu}\right)^{(\nu+1)/2}} \,. \tag{H.10}$$

This, obviously, is Student's or Gosset's density for the random variable

$$T(\nu) = \frac{X-\mu}{S} \,. \tag{H.11}$$

Due to (H.3) and (H.7), the number of degrees of freedom is $\nu = n-1$.

Variable $T(\nu) = \dfrac{\bar{X}-\mu}{S/\sqrt{n}}$

Let us replace (H.4) by

$$\bar{x} = \mu + ts/\sqrt{n} \tag{H.12}$$

in which

$$\bar{x} = \frac{1}{n}\sum_{l=1}^{n} \bar{x}_l \tag{H.13}$$

denotes the sample mean. As

[1] Averaging by $p_S(s)$ leads to the same result as $p_S(s)ds = p_{S^2}(S^2)dS^2$.

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

we have

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

Substituting $\eta = (\bar{x} - \mu)/(\sigma/\sqrt{n})$ leads us back to (H.6). Hence, the random variable

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

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

I Uncertainty Band Versus EP-Region

The fitting of straight lines asks for two-dimensional uncertainty regions. Remarkably enough, there are two different, however, equivalent approaches [29].

Set of Straight Lines Versus Set of 2-Tuples

Consider a straight line as defined by a 2-tuple of true values

$$\begin{pmatrix} \beta_{0,1} \\ \beta_{0,2} \end{pmatrix}$$

pegging its ordinate intercept $\beta_{0,1}$ and slope $\beta_{0,2}$. The least squares adjustment provides a pair of estimators

$$\begin{pmatrix} \bar{\beta}_1 \\ \bar{\beta}_2 \end{pmatrix}$$

devising a straight line

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

However, there are still other straight lines compatible with the error model and the input data. The idea is to engird this bunch by an uncertainty band

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

We expect the upper and lower borderlines

$$\bar{y}(x) + u_{\bar{y}(x)} \quad \text{and} \quad \bar{y}(x) - u_{\bar{y}(x)}$$

to localize the true straight line.

At the same time, the fitted straight line may be endowed by a confidence ellipse and a security polygon. Their piecing together devises an EP-region. The latter marks a set of tuples (β_1, β_2) being compatible with the input data and the error model. We expect the 2-tuple of true values, $(\beta_{0,1},\, \beta_{0,2})$, to be an element of this set.

The approaches, though ostensibly different, should put forth concurrent results: The set of straight lines, as devised by the uncertainty band $\bar{y}(x) \pm u_{\bar{y}(x)}$ should reproduce the set of 2-tuples $(\beta_1,\, \beta_2)$ as confined by the EP-region, and vice versa.

We shall establish this complementarity. To this end, we step back and decompose the uncertainty band and the EP-region into its components due to random and systematic errors.

Transformation Procedures

Initially, we transform the random share of the uncertainty band into the confidence ellipsoid and, thereafter, the systematic share into the security polygon.

Random Errors

Consider case (i) as quoted in Table 12.1. Abstaining from systematic errors, the uncertainty band is given by (13.26) disregarding the term $f_{s,y}$. The confidence ellipse is given in (13.27).

We envisage the set of tangents to the upper and lower boundaries of the uncertainty band. Each tangent specifies a certain y-intercept and slope, i.e a tuple

$$\begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} .$$

Considering Fig. I.1, we see the parameters β_1, β_2 of the tangent to P_1 to reproduce the point P_1^* on the ellipse. More general, a tangent gliding from P_1 via P_2 to P_3 is seen to establish the right arc P_1^*, P_2^*, P_3^* of the confidence ellipse. Similarly, a tangent gliding from P_5 via P_6 to P_7 is seen to reproduce the ellipse's left arc P_5^*, P_6^*, P_7^* .

Let us specify the differences $\beta_1 - \bar{\beta}_1$ and $\beta_2 - \bar{\beta}_2$. For this, we denote the upper boundary of the uncertainty band by

$$\begin{aligned} y_2(x) &= \bar{y}(x) + u_{\bar{y}(x)} \\ &= \bar{\beta}_1 + \bar{\beta}_2\, x + t_P(m-2)\, s_y \sqrt{\sum_{i=1}^{m} (b_{i1} + b_{i2}\, x)^2} \, . \end{aligned} \tag{I.1}$$

Due to (13.17) we observe

$$y_2(x) = \bar{\beta}_1 + \bar{\beta}_2\, x + t_P(m-2) \sqrt{s_{\bar{\beta}_1 \bar{\beta}_1} + 2 s_{\bar{\beta}_1 \bar{\beta}_2}\, x + s_{\bar{\beta}_2 \bar{\beta}_2} x^2} \, . \tag{I.2}$$

The tangent to any point $(x, y_2(x))$

$$y(\xi) = y_2(x) + y_2'(x)(\xi - x) = \beta_1 + \beta_2\,\xi \tag{I.3}$$

implies

$$\beta_1 = y_2(x) - y_2'(x)\,x \quad \text{and} \quad \beta_2 = y_2'(x)\,.$$

With

$$y_2'(x) = \bar\beta_2 + t_P(m-2)\frac{s_{\bar\beta_1\bar\beta_2} + s_{\bar\beta_2\bar\beta_2}\,x}{\sqrt{s_{\bar\beta_1\bar\beta_1} + 2s_{\bar\beta_1\bar\beta_2}\,x + s_{\bar\beta_2\bar\beta_2}x^2}} \tag{I.4}$$

we have

$$\beta_1 - \bar\beta_1 = t_P(m-2)\frac{s_{\bar\beta_1\bar\beta_1} + s_{\bar\beta_1\bar\beta_2}\,x}{\sqrt{s_{\bar\beta_1\bar\beta_1} + 2s_{\bar\beta_1\bar\beta_2}\,x + s_{\bar\beta_2\bar\beta_2}x^2}}\,. \tag{I.5}$$

Similarly, we find

$$\beta_2 - \bar\beta_2 = t_P(m-2)\frac{s_{\bar\beta_1\bar\beta_2} + s_{\bar\beta_2\bar\beta_2}\,x}{\sqrt{s_{\bar\beta_1\bar\beta_1} + 2s_{\bar\beta_1\bar\beta_2}\,x + s_{\bar\beta_2\bar\beta_2}x^2}}\,. \tag{I.6}$$

Ultimately, inserting (I.5) and (I.6) into (13.27) and gathering terms in powers of x^0, x^1, and x^2 issues an identity, provided that

$$t_P(m-2) = t_P(2, m-2)\,.$$

This, however, ascertains differing probabilities as

$$P(m-2) \neq P(2, m-2)\,. \tag{I.7}$$

The disparity is to be attributed to the observation that the straight line's uncertainty band is established by Student's density, which is one-dimensional, while the confidence ellipse is issued by Hotelling's density, which is two-dimensional. To have an example, we assume $m = 14$ and choose $P(2, m-2) = 95\%$ for Hotelling's density. This produces $t_P(2, m-2) = 3.0$. On the other hand, for $t_P(m-2) = 3.0$, Student's density issues a probability of $P(m-2) = 99\%$.

Letting x tend to infinity, we get the tangent to $y_2(x)$ with y-intercept and slope

$$\begin{aligned} \lim_{x\to\infty}\{\beta_1\} &= \bar\beta_1 + t_P(m-2)\frac{s_{\bar\beta_1\bar\beta_2}}{\sqrt{s_{\bar\beta_2\bar\beta_2}}} \\ \lim_{x\to\infty}\{\beta_2\} &= \bar\beta_2 + t_P(m-2)\frac{s_{\bar\beta_2\bar\beta_2}}{\sqrt{s_{\bar\beta_2\bar\beta_2}}} \end{aligned} \tag{I.8}$$

producing the point P_4^* of Fig. I.1. Putting $x = 0$, we find the tangent to $y_2(x)$ with y-intercept and slope

$$\begin{aligned}\beta_1 - \bar{\beta}_1 &= t_P(m-2)\frac{s_{\bar{\beta}_1\bar{\beta}_1}}{\sqrt{s_{\bar{\beta}_1\bar{\beta}_1}}} \\ \beta_2 - \bar{\beta}_2 &= t_P(m-2)\frac{s_{\bar{\beta}_1\bar{\beta}_2}}{\sqrt{s_{\bar{\beta}_1\bar{\beta}_1}}}\,.\end{aligned} \tag{I.9}$$

We observe (I.8) to coincide with (D.2) and (I.9) with (D.1). Deriving corresponding expressions for the lower boundary of the uncertainty band

$$\begin{aligned}y_1(x) &= \bar{y}(x) - u_{\bar{y}(x)} \\ &= \bar{\beta}_1 + \bar{\beta}_2\,x - t_P(m-2)\,s_y\sqrt{\sum_{i=1}^{m}(b_{i1}+b_{i2}\,x)^2}\end{aligned} \tag{I.10}$$

produces

$$\begin{aligned}\beta_1 - \bar{\beta}_1 &= -t_P(m-2)\frac{s_{\beta_1\beta_1} + s_{\beta_1\beta_2}\,x}{\sqrt{s_{\beta_1\beta_1} + 2s_{\beta_1\beta_2}\,x + s_{\beta_2\beta_2}x^2}} \\ \beta_2 - \bar{\beta}_2 &= -t_P(m-2)\frac{s_{\beta_1\beta_2} + s_{\beta_2\beta_2}\,x}{\sqrt{s_{\beta_1\beta_1} + 2s_{\beta_1\beta_2}\,x + s_{\beta_2\beta_2}x^2}}\end{aligned} \tag{I.11}$$

For $x \to \infty$, we obtain the tangent to $y_1(x)$ with y-intercept and slope

$$\begin{aligned}\lim_{x\to\infty}\{\beta_1\} &= \bar{\beta}_1 - t_P(m-2)\frac{s_{\bar{\beta}_1\bar{\beta}_2}}{\sqrt{s_{\bar{\beta}_2\bar{\beta}_2}}} \\ \lim_{x\to\infty}\{\beta_2\} &= \bar{\beta}_2 - t_P(m-2)\frac{s_{\bar{\beta}_2\bar{\beta}_2}}{\sqrt{s_{\bar{\beta}_2\bar{\beta}_2}}}\end{aligned} \tag{I.12}$$

establishing the point P_8^* of Fig. I.1.

Vice versa, we might wish to deploy the coordinates β_1 and β_2 of the ellipse's circumference directly as given in (13.27) and draw a bunch of straight lines

$$y(x) = \beta_1 + \beta_2\,x$$

in-between the upper and lower borders of the straight line's uncertainty band. We in fact find the bunch to fit the uncertainty band, given we boost Student's t from $t_P(m-2)$ up to Hotelling's $t_P(2, m-2)$ putting $t_P(m-2) = t_P(2, m-2)$. Otherwise, the bunch would exceed the borderlines of the uncertainty band.

Case (ii), as specified in Table 12.1, leads to a corresponding result, here, however, we have to put

$$t_P(n-1) = t_P(2, n-1)\,.$$

Systematic Errors

To illustrate the proceeding, we address case (ii) of Table 12.1 ignoring random errors. To simplify the discussion, the number of measuring points is reduced to just three. On its left, Fig. I.2 displays the least squares line and its uncertainty band. On the right we observe the associated security polygon. The symbols LS_1 to LS_6 designate the line segments of the upper and lower borderlines of the uncertainty band.

Intuitively, we expect the y-intercept and slope of line segment LS_1 to reproduce the polygon's vertex V_1; furthermore, segment LS_2 to reproduce vertex V_2 and, finally, segment LS_3 vertex to issue V_3. Corresponding relations should hold with respect to the segments of the upper borderline and the polygon's remaining three vertices. To keep track of the supposed relationships, we resort to a numerical example,

$$\boldsymbol{B} = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \\ b_{31} & b_{32} \end{pmatrix} = \begin{pmatrix} 1.33 & -0.50 \\ 0.33 & 0.00 \\ -0.67 & 0.50 \end{pmatrix} .$$

Referring to (14.21)

$$f_{s,\bar{y}(x)} =\mid b_{11} + b_{12}x \mid f_{s,\bar{y}_1} + \mid b_{21} + b_{22}x \mid f_{s,\bar{y}_2} + \mid b_{31} + b_{32}x \mid f_{s,\bar{y}_3} \, ,$$

we have

$$LS_1 : x < -\frac{b_{31}}{b_{32}}; \quad LS_2 : -\frac{b_{31}}{b_{32}} \le x < -\frac{b_{11}}{b_{12}}; \quad LS_3 : x \ge -\frac{b_{11}}{b_{12}} \, . \tag{I.13}$$

Regarding LS_1, the propagated systematic error is given by

$$\begin{aligned} f_{s,\bar{y}(x)} &= (b_{11} + b_{12}x) f_{s,\bar{y}_1} + b_{21} f_{s,\bar{y}_2} - (b_{31} + b_{32}x) f_{s,\bar{y}_3} \\ &= (b_{11} f_{s,\bar{y}_1} + b_{21} f_{s,\bar{y}_2} - b_{31} f_{s,\bar{y}_3}) + (b_{12} f_{s,\bar{y}_1} - b_{32} f_{s,\bar{y}_3})\, x \, . \end{aligned} \tag{I.14}$$

Hence, segment LS_1

$$\begin{gathered} \bar{y}(x) - f_{s,\bar{y}(x)} = \bar{\beta}_1 + \bar{\beta}_2 \, x \\ -(b_{11} f_{s,\bar{y}_1} + b_{21} f_{s,\bar{y}_2} - b_{31} f_{s,\bar{y}_3}) - (b_{12} f_{s,\bar{y}_1} - b_{32} f_{s,\bar{y}_3})\, x \end{gathered} \tag{I.15}$$

has y-intercept and slope

$$\begin{aligned} \beta_1 &= \bar{\beta}_1 - (b_{11} f_{s,\bar{y}_1} + b_{21} f_{s,\bar{y}_2} - b_{31} f_{s,\bar{y}_3}) \\ \beta_2 &= \bar{\beta}_2 - (b_{12} f_{s,\bar{y}_1} - b_{32} f_{s,\bar{y}_3}) \, . \end{aligned} \tag{I.16}$$

We suppose the pair β_1, β_2 to reproduce the polygon's upper leftmost vertex V_1. To show this, we turn to Appendix F. Indeed, rewriting (14.10),

$$\begin{aligned} f_{\bar{\beta}_1} &= b_{11} f_{\bar{y}_1} + b_{21} f_{\bar{y}_2} + b_{31} f_{\bar{y}_3} \\ f_{\bar{\beta}_2} &= b_{12} f_{\bar{y}_1} \qquad\qquad + b_{32} f_{\bar{y}_3} \,, \end{aligned} \tag{I.17}$$

and putting

$$f^*_{\bar{y}_1} = \text{sign}(b_{12}) f_{s,\bar{y}_1} ; \quad f^*_{\bar{y}_3} = \text{sign}(b_{32}) f_{s,\bar{y}_3}$$

we find

$$\begin{aligned} f_{s,\bar{\beta}_1} &= b_{11}\text{sign}(b_{12}) f_{s,\bar{y}_1} - b_{21} f_{s,\bar{y}_2} + b_{31}\text{sign}(b_{32}) f_{s,\bar{y}_3} \\ f_{s,\bar{\beta}_2} &= b_{12}\text{sign}(b_{12}) f_{s,\bar{y}_1} + b_{32}\text{sign}(b_{32}) f_{s,\bar{y}_3} \end{aligned}$$

or

$$\begin{aligned} f_{s,\bar{\beta}_1} &= -b_{11} f_{s,\bar{y}_1} - b_{21} f_{s,\bar{y}_2} + b_{31} f_{s,\bar{y}_3} \\ f_{s,\bar{\beta}_2} &= -b_{12} f_{s,\bar{y}_1} + b_{32} f_{s,\bar{y}_3} \end{aligned} \tag{I.18}$$

As the polygon is centered in $(\bar{\beta}_1, \bar{\beta}_2)$, (I.18) coincides with (I.16) as it should be.

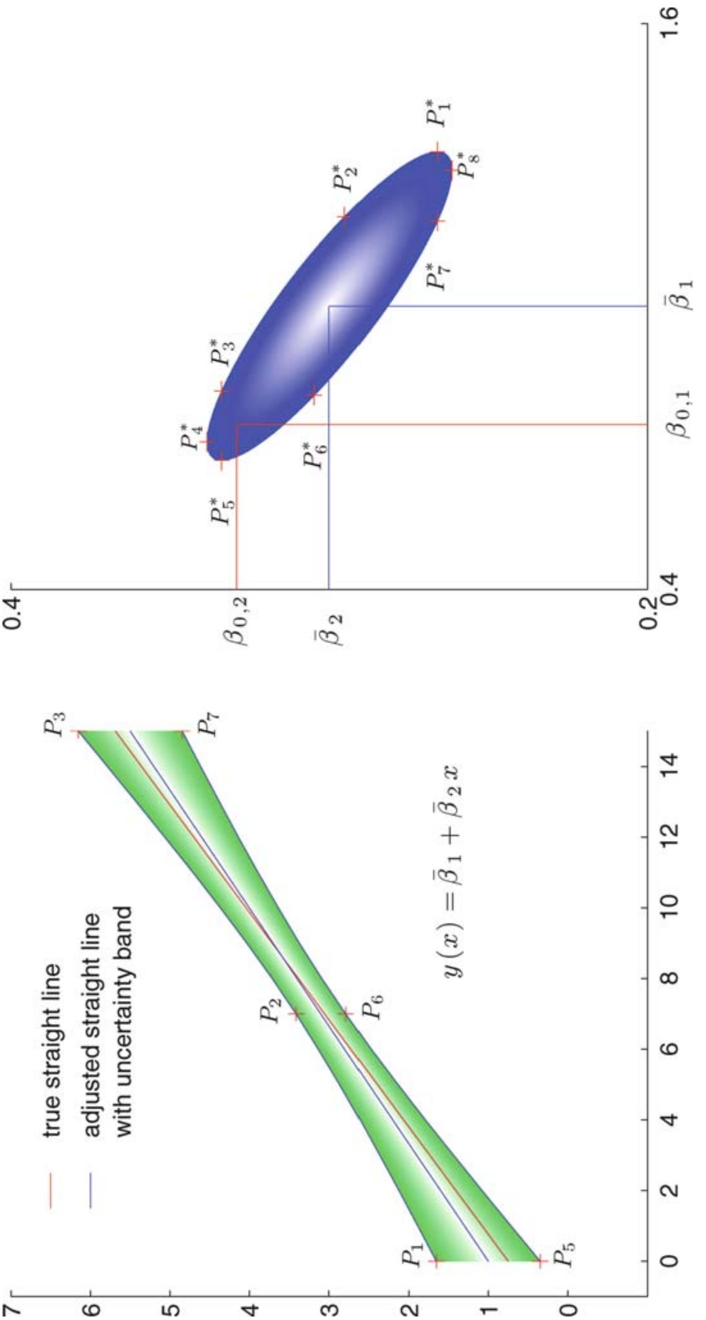

Fig. I.1. Random share of uncertainty band versus confidence ellipse

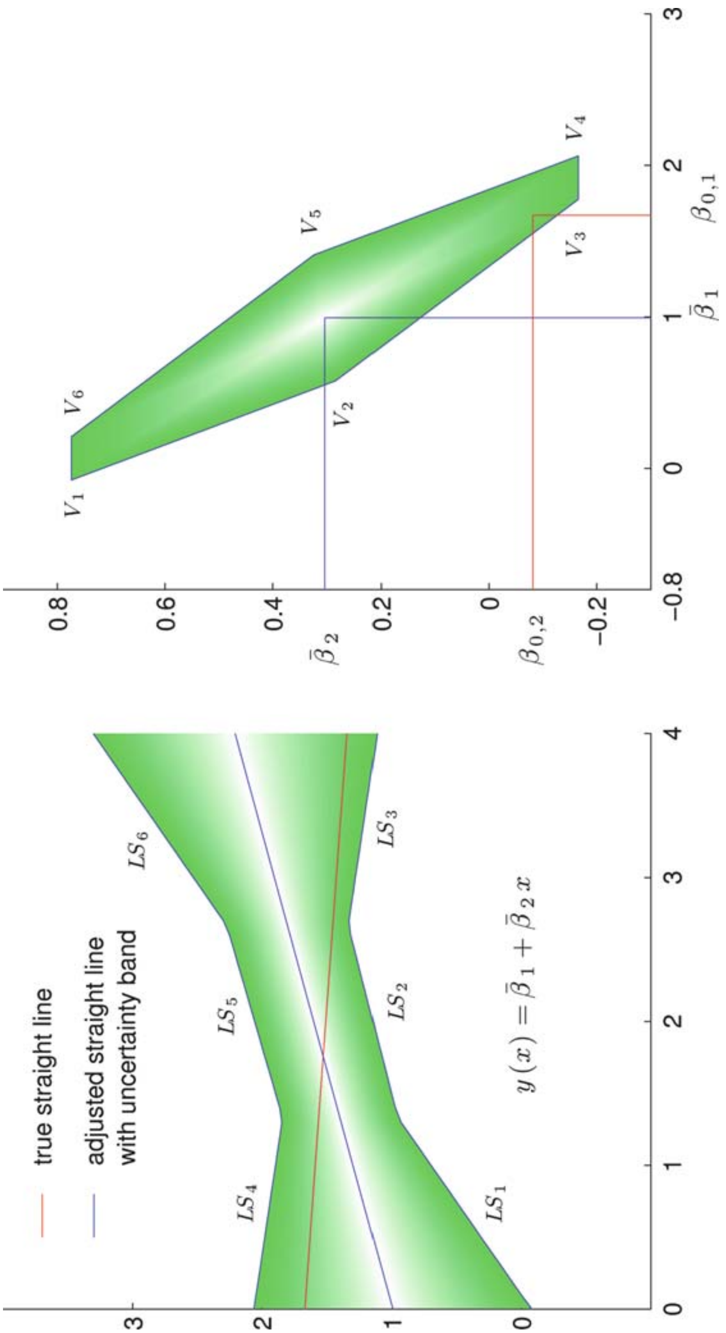

Fig. I.2. Systematic proportion of uncertainty band versus security polygon

J Quantiles of Hotelling's Density

$t_{0.95}$; 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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Index