Uncertainties and Covariances
-
basic concepts and procedures

a collection of transparencies for use in a lecture course by

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1. Introduction

a simple example:

Given two samples of a certain radioisotope to be used as relative radiation sources for instrument testing.

Available information:

sample 1 counts	900
sample 2 counts	981
background	700

Question:

Calculate the ratio of the net source activities, including its uncertainty.

All terms and definitions based on

1. VIM (1984): ***International vocabulary of basic and general terms in metrology*** published jointly by ISO/IEC/OIML/BIPM

2. "The Guide": ***Guide to the expression of uncertainty in measurement***, (developed jointly by BIPM, IEC, IFCC, ISO, IUPAC, OIML), ISO/TAG 4/WG 3
published in bookform by the International Organization for Standardization, Geneva, Switzerland (2 nd edition 1995).

Many of the recommendations therein are available on the Internet, e.g. at

http://physics.nist.gov/Pubs/guidelines/

a few clarifications, concerning frequently used terms

error:

the deviation of the result of a particular measurement from the *unknown "true value"* of the measurand

errors may be due to

- incorrect human working methods, which could be traced by thoroughly considering the whole measurement procedure
- non-perfect, non-ideal instrument behavior, or
- fluctuations due to physical phenomena

uncertainty:

a parameter, associated with the result of a measurement, that characterizes the dispersion of the values that could reasonably be attributed to the measurand

deviations, for which the algebraic sign and magnitude are unknown and fluctuating, leading to *scatter* in the results of a measurement:

random (statistical) errors

deviations, which *influence a series of measurements* in the same way and in the same, but unknown direction, yielding a *shift* in the results:

"systematic" (correlated) errors

accuracy of measurement:

closeness of the agreement between the result of a measurement and the value of the measurand.

repeatability (of results of measurements):

closeness of the agreement between the results of successive measurements of the same measurand carried out under the same conditions of measurement.

reproducibility (of results of measurements):

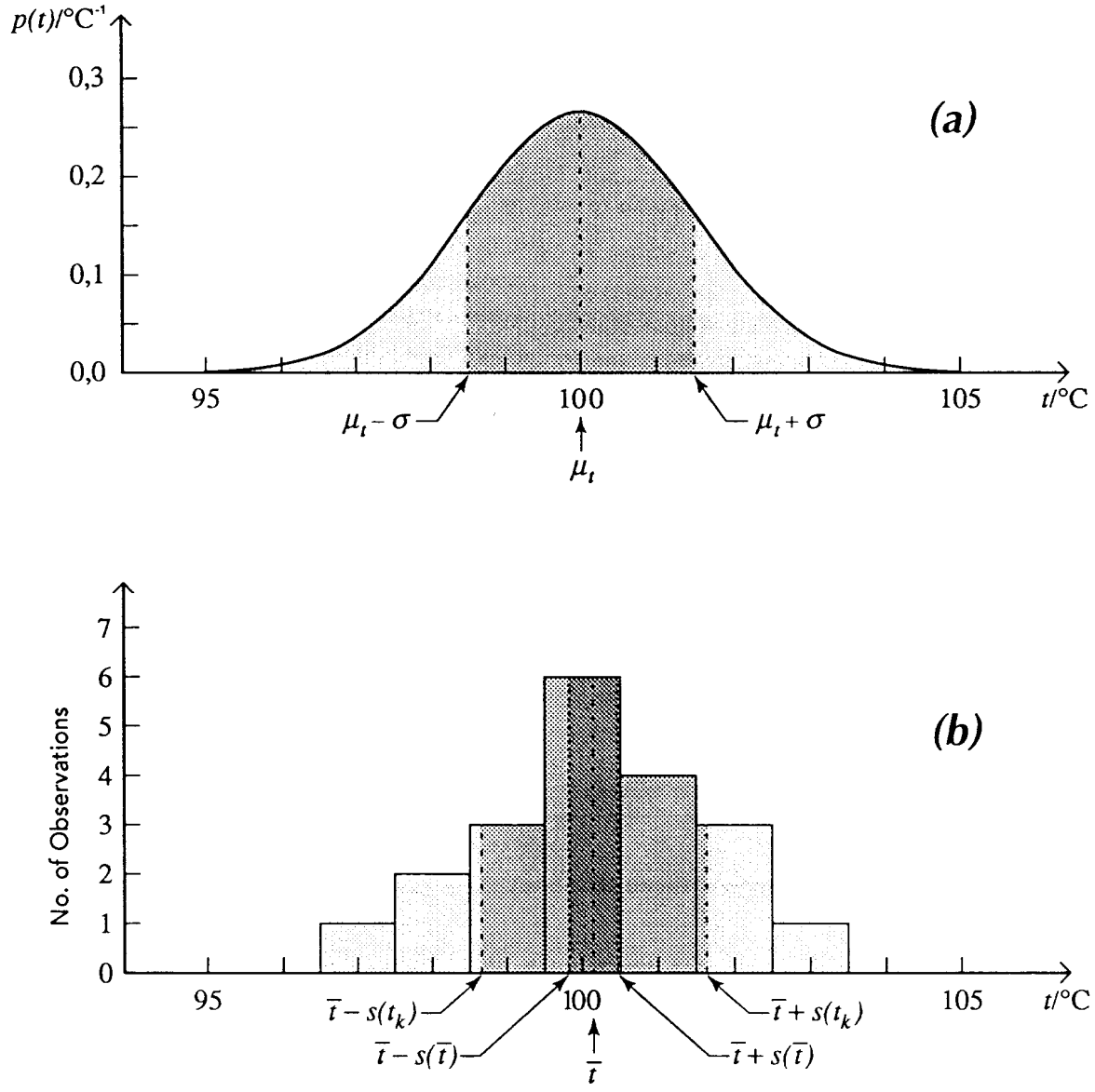
closeness of the agreement between the results of measurements of the same measurand carried out under changed conditions of measurement.

2. Evaluation of measurement uncertainties:

2.1. Type A (evaluation of uncertainties)

=: components of uncertainty evaluated by statistical methods

Figure 1. Graphical illustration of evaluating the standard uncertainty of an input quantity from repeated observations



Let x be a random variable and t a parameter,
then the **distribution function** F(t) is defined as

$$F(t) = P(x < t) \qquad \text{for } -\infty < t < \infty$$

and the derivative

$$f(t) = dF(t) / dt \; = \; F'(t)$$

is called the **probability density function**

If we know the probability density function p(z) for a random variable z, we can calculate the expectation or mean value of the variable

$$E(z) \; = \; \mu_z \; = \; \int z \; p(z) \; dz$$

and its variance

$$\sigma^2 (z) \; = \; \int (z - \mu_z)^2 \; p(z) \; dz$$

The positive square root of the variance, σ (z), is called the **standard deviation** of a measurement and is generally quoted as **standard uncertainty**.
For a given probability density function this determines a **confidence level** for the result of the measurement = a probability that the "true value" lies within a given interval around the mean.

for a normal or Gauss distribution this means

for an interval $x \pm k \, \sigma(x)$	the probability is
k = 1.00	68.30%
k = 2.00	95.45%
k = 3.00	99.73%
k = 1.64	90%
k = 1.96	95%
k = 2.58	99%

Statistical estimate of uncertainty from repeated observations of the same quantity:

$$\langle z \rangle = m_z = \frac{1}{n}\sum_{i=1}^{n} z_i$$

with a variance of the individual observations

$$s^2(z_i) = \frac{1}{n-1}\sum_{i=1}^{n}\left(z_i - m_z\right)^2$$

and a variance of the average

$$s^2(m_z) = \frac{1}{n(n-1)}\sum_{i=1}^{n}\left(z_i - m_z\right)^2$$

the positve square root of which is taken as standard uncertainty:

$$u(m_z) = \sqrt{s^2(m_z)} = s(z_i)/\sqrt{n}$$

2.2. Type B (evaluation of uncertainties)

Method of evaluation of a standard uncertainty $u(x_i)$ by means other than the statistical analysis of a series of observations.

Judgement using all relevant information on the possible variability of x_i. The pool of information may include

- previous measurement data
- experience with or general knowledge of the behavior and properties of relevant materials and instruments
- manufacturers specifications
- uncertainties assigned to reference data taken from handbooks
- data provided in calibration and other certificates

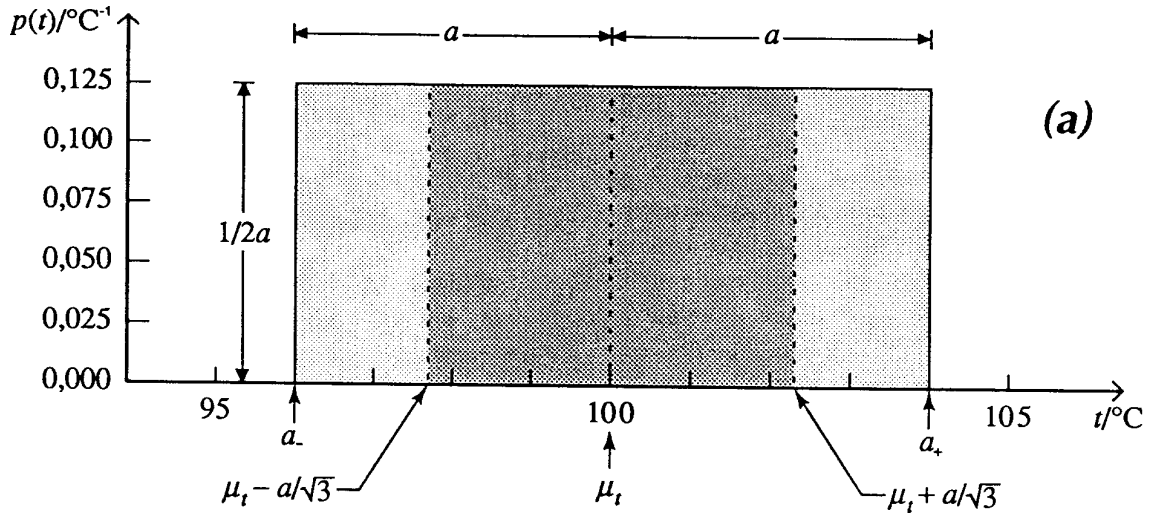
Proper use of the pool of available information calls for insight based on experience and general knowledge.

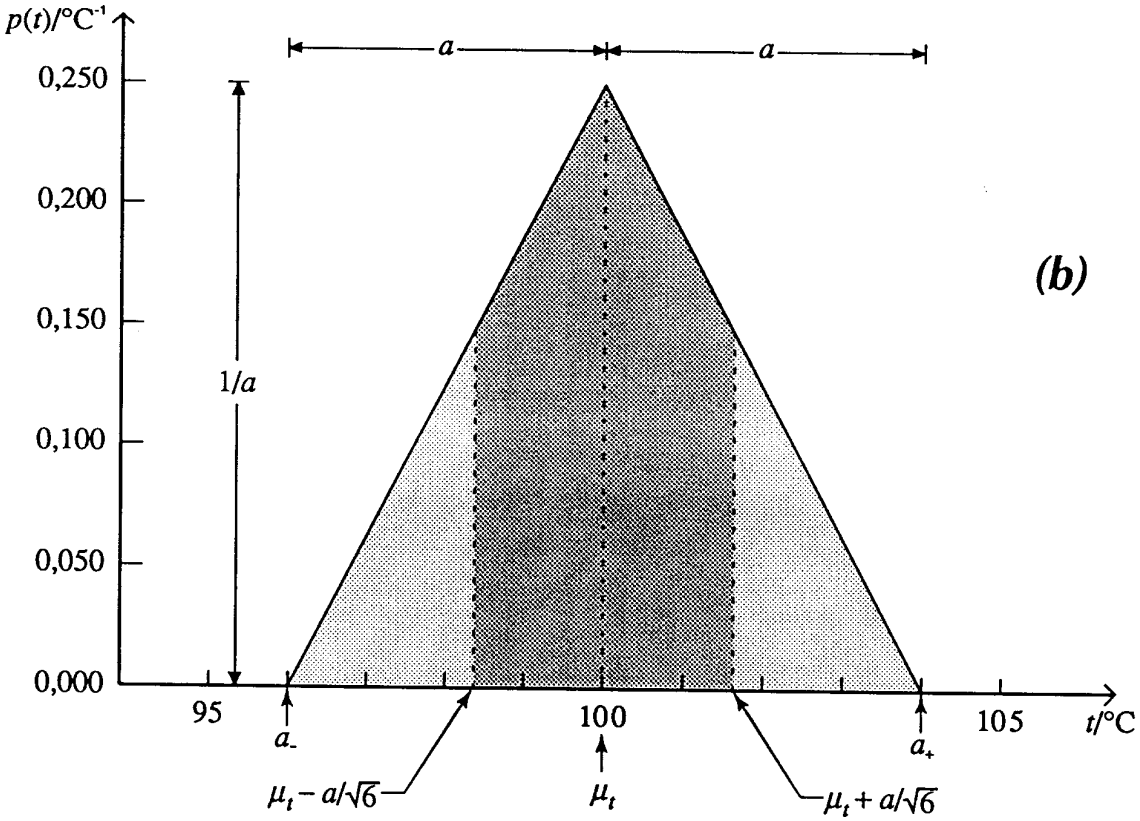
A type B evaluation of standard uncertainty can be as reliable as a type A evaluation, especially in a measurement situation, where a type A evaluation is based on a small number of statistically independent observations.

relative standard deviation of the experimental standard deviation of the mean of a sample of n observations (assumed normal distribution)

# of observations n	rel. standard dev. (%)
2	76
3	52
4	42
5	36
10	24

If reasonable assumptions on the distribution of the measurements around an estimated mean can be made, e.g. equal probability between some upper and lower bound or triangular probability around the mean, it is also possible to determine a standard uncertainty with a similar confidence level than in a type A evaluation with assumption of normally distributed measurement results.





2.3. Determining combined standard uncertainty:

If y is a function F of several independent observable quantities x_k

$$y = F(x_1, x_2, ..., x_k)$$

the **combined standard uncertainty** of the estimate y is designated $u_c(y)$ and is the positive square root of the combined variance $u_c^2(m_y)$ obtained from

$$u_c^2(m_y) = \sum_{i=1}^{k} \left(\frac{\partial F}{\partial x_i} \right)^2 u^2(m_{x_i})$$

which is also known as the *law of propagation of uncertainty.*
The partial derivatives $\delta F/\delta x_i$ describe, how the output estimate y varies with changes in the values of the input estimates x_i and are therefore often referred to as **sensitivity coefficients**.

in particular, we get for a linear combination of variables

$y = ax_1 + bx_2 + cx_3$

$u^2(m_y) = a^2\, u^2(m_{x1}) + b^2\, u^2(m_{x2}) + c^2\, u^2(m_{x3})$

for a product of variables

$y = a\, x_1\, x_2\, x_3$

$$\frac{u^2(m_y)}{m_y{}^2} = \frac{u^2(m_{x1})}{m_{x1}{}^2} + \frac{u^2(m_{x2})}{m_{x2}{}^2} + \frac{u^2(m_{x3})}{m_{x3}{}^2}$$

and for some more elementary functions

function	variance
$y = ax + b$	$u^2(m_y) = a^2\, u^2(m_x)$
$y = ax_1 + bx_2$	$u^2(m_y) = a^2\, u^2(m_{x1}) + b^2\, u^2(m_{x2})$
$y = ax^n$	$u^2(m_y) / m_y^2 = n^2\ u^2(m_x) / m_x^2$
$y = \ln(x)$	$u^2(m_y) = u^2(m_x) / m_x^2$
$y = \ln(x_1 + x_2)$	$u^2(m_y) = [u^2(m_{x1}) + u^2(m_{x2})] / (m_{x1} + m_{x2})^2$
$y = \ln(x_1/x_2)$	$u^2(m_y) = u^2(m_{x1}) / m_{x1}^2 + u^2(m_{x2}) / m_{x2}^2$

Two random variables with possible dependencies

$\sigma^2(z) = \int (z - \mu_z)^2 \, p(z)\, dz$ was defined as variance

$\iint (y - m_y)(z - m_z)\, p(y,z)\, dy\, dz =:$ **cov(y,z)** $= \mathrm{cov}(z,y)$

is defined as **covariance**, which gives a measure of the mutual dependency of the two random variables y and z.

an estimate may be obtained from n repeated simultaneous observations of y and z:

$$s(y_i, z_i) = \frac{1}{n-1} \sum_{i=1}^{n} (y_i - m_y)(z_i - m_z)$$

For convenience often a relative quantity named correlation coefficient is used:

$$\rho(y, z) = \mathrm{cov}(y, z) / \sigma(y)\, \sigma(z)$$

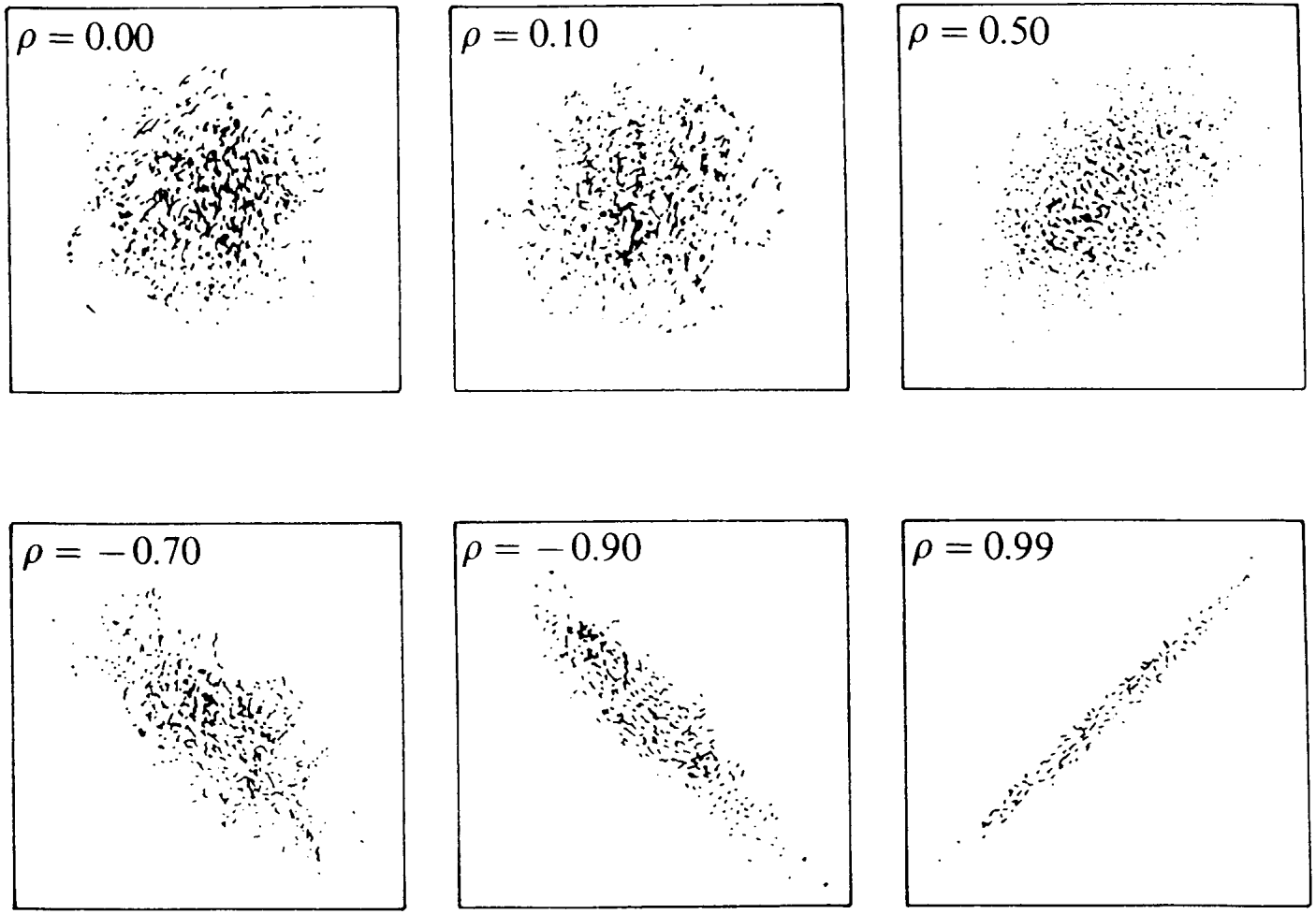
with the estimate

$$r(y_i, z_i) = s(y_i, z_i) / s(y_i)\, s(z_i)$$

These coefficients are pure numbers in the range –1 to +1 inclusive.

ρ positive if $y > m_y$ and $z > m_z$, or $y < m_y$ and $z < m_z$ appear together

ρ negative if $y < m_y$ and $z > m_z$, or $y > m_y$ and $z < m_z$ on the average



Scatter plots showing examples of different degrees of correlation

For the case of existing correlation the formula for determining the combined standard uncertainty has to be generalized. The appropriate expression is

$$u_c^{\,2}(y) = \sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\partial F}{\partial x_i}\frac{\partial F}{\partial x_j}u(x_i, x_j)$$

$$= \sum_{i=1}^{n}\left(\frac{\partial F}{\partial x_i}\right)^2 u^2(x_i) + 2\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\frac{\partial F}{\partial x_i}\frac{\partial F}{\partial x_j}u(x_i, x_j)$$

for some frequently needed simple functions this leads to

$u^2(a)$	=	0
$u^2(a+x)$	=	$u^2(x)$
$u^2(ax)$	=	$a^2\, u^2(x)$
$u^2(x + y)$	=	$u^2(x) + u^2(y) + 2\, \mathrm{cov}(x, y)$
$u^2(x - y)$	=	$u^2(x) + u^2(y) - 2\, \mathrm{cov}(x, y)$

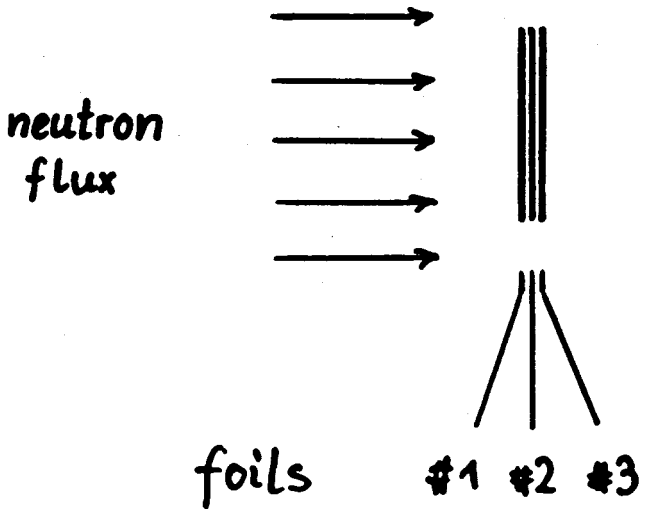
$$\frac{u^2(x\times y)}{(x\times y)^2} = \frac{u^2(x)}{x^2} + \frac{u^2(y)}{y^2} + \frac{2\,\mathrm{cov}(x\times y)}{x\times y}$$

$$\frac{u^2(x/y)}{(x/y)^2} = \frac{u^2(x)}{x^2} + \frac{u^2(y)}{y^2} - \frac{2\,\mathrm{cov}(x\times y)}{x\times y}$$

$\mathrm{cov}(a+x, b+y)$	=	$\mathrm{cov}(x, y)$
$\mathrm{cov}(ax,by)$	=	$a\, b\, \mathrm{cov}(x, y)$
$\mathrm{cov}(x, x+y)$	=	$u^2(x) + \mathrm{cov}(x, y)$
$\mathrm{cov}(x, x-y)$	=	$u^2(x) - \mathrm{cov}(x, y)$
$\mathrm{cov}(x+y, x-y)$	=	$u^2(x) - u^2(y)$
$\mathrm{cov}(x+y, x+y)$	=	$u^2(x) + u^2(y) + 2\, \mathrm{cov}(x, y)$
$\mathrm{cov}(x-y, x-y)$	=	$u^2(x) + u^2(y) - 2\, \mathrm{cov}(x, y)$

Example 2:

3 neutron cross sections of different materials have been determined by simultaneous irradiation of 3 foils in a common neutron field



and subsequent measurement of the induced radioactivity by a suitable γ-detector. The number of counts c is determined by

$$c = N * \sigma * \phi * \varepsilon * f$$

consequently we can calculate the cross section σ as

$$\sigma = c / (N * \phi * \varepsilon * f)$$

We want to calculate the uncertainty of the ratio σ_1/σ_2 and the product $\sigma_1 * \sigma_2$. For simplicity we assume no uncertainty in N and in f.

From a type A evaluation of standard uncertainties we get the results for the individual components of uncertainty contributing to the combined standard uncertainty of the cross sections. Because the cross sections are calculated from a product of input quantities the following table summarizes the relative standard uncertainties.

component of uncertainty	foil # ->	1	2	3
c		0.5 %	1.0 %	0.3 %
ε		1.6 %	2.2 %	1.3 %
ϕ		2.0 %	2.0 %	2.0 %

due to the common calibration of the γ-detector the efficiencies for the respective γ-transitions are partly correlated:

$(\varepsilon_1, \varepsilon_2) = 80\ \%$, $(\varepsilon_1, \varepsilon_3) = 50\ \%$, $(\varepsilon_2, \varepsilon_3) = 60\ \%$

as the components for each individual cross section are not correlated we can calculate the respective standard uncertainties by simply adding the variances and taking the positive square root:

	$u^2(x_i)$ %²	$u_c^2(\sigma_i)$ %²	$u_c(\sigma_i)$
σ_1	$0.5^2 + 1.6^2 + 2.0^2$	6.81	2.61 %
σ_2	$1.0^2 + 2.2^2 + 2.0^2$	9.84	3.14 %
σ_3	$0.3^2 + 1.3^2 + 2.0^2$	5.78	2.40%

Taking just these uncertainties, we would get

$$u(\sigma_1/\sigma_2) = u(\sigma_1 * \sigma_2) = \sqrt{u_c^2(\sigma_1) + u_c^2(\sigma_2)}$$
$$= \sqrt{6.81 + 9.84} = 4.08\ \%$$

but we have correlation due to ϕ which is fully correlated and ε with partial correlation. Consequently we get

	cov (σ_i, σ_j) by components	cov (σ_i, σ_j)
cov (σ_1, σ_2)	$1.6 * 2.2 * 0.8 + 2.0 * 2.0$	6.82 %²
cov (σ_1, σ_3)	$1.6 * 1.3 * 0.5 + 2.0 * 2.0$	5.05 %²
cov (σ_2, σ_3)	$2.2 * 1.3 * 0.6 + 2.0 * 2.0$	5.72 %²

hence the correct results are

$$u(\sigma_1 * \sigma_2) = \sqrt{u_c^2(\sigma_1) + u_c^2(\sigma_2) + \mathbf{2\ cov\ (\sigma_1, \sigma_2)}}$$
$$= 5.50\ \%$$

$$u(\sigma_1/\sigma_2) = \sqrt{u_c^2(\sigma_1) + u_c^2(\sigma_2) - \mathbf{2\ cov\ (\sigma_1, \sigma_2)}}$$
$$= 1.74\ \%$$

The outlined calculation (and representation) procedure is only practical for a small number of input quantities and/or evaluation results. As can be seen already from the above tables the whole problem is ideally suited for matrix representation:

The (relative) variances and covariances can be arranged as

$$V = \begin{pmatrix} 6.81 & & \\ 6.82 & 9.84 & \\ 5.04 & 5.72 & 5.78 \end{pmatrix}$$

from where all desired quantities can be calculated easily

$$u_c(\sigma_i)/\sigma_i = \sqrt{\mathbf{V}_{ii}} \qquad r_{ij} = \frac{\mathbf{V}_{ij}}{\sqrt{\mathbf{V}_{ii}\mathbf{V}_{jj}}}$$

so the final result could be given as

$$\begin{array}{ll} \sigma_1 & \pm 2.61\ \% \\ \sigma_2 & \pm 3.14\ \% \\ \sigma_3 & \pm 2.40\ \% \end{array} \qquad \begin{pmatrix} 1.00 & & \\ 0.83 & 1.00 & \\ 0.80 & 0.76 & 1.00 \end{pmatrix}$$

3. General form for deriving combined standard uncertainties by matrix formalism.

If all output quantities $y_1, y_2, \ldots y_k, \ldots y_m$ (combined in a vector **y**) are a linear combination of the $x_1, x_2, \ldots x_i, \ldots x_n$ (combined in a vector **x)**, the $(m \times 1)$ column vector **y** is related to the $(n \times 1)$ vector **x** by a linear transformation

$$\mathbf{y} = \mathbf{T}\,\mathbf{x} + \mathbf{a}$$

and the corresponding covariance matrices $\mathbf{C_x}$ and $\mathbf{C_y}$ transform according to

$$\mathbf{C_y} = \mathbf{T}\,\mathbf{C_x}\,\mathbf{T}^t$$

with **T** being the transformation matrix of dimension $(m \times n)$ and $\mathbf{T}^t$ its transpose.

Our introductory example then would appear in the following notation:

Input variables G_1, G_2, B
output variables N_1, N_2

the relationship reads:

$$N_1 = 1 * G_1 + 0 * G_2 - B$$
$$N_2 = 0 * G_1 + 1 * G_2 - B$$

so the transformation matrix T becomes

$$T = \left(\begin{array}{ccc} 1 & 0 & -1 \\ 0 & 1 & -1 \end{array}\right)$$

and the input covariance matrix is

$$C_x = \begin{pmatrix} 900 & 0 & 0 \\ 0 & 981 & 0 \\ 0 & 0 & 700 \end{pmatrix} \qquad T^t = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ -1 & -1 \end{pmatrix}$$

$$T \times C_x = \begin{pmatrix} 900 & 0 & -700 \\ 0 & 981 & -700 \end{pmatrix}$$

$$T \times C_x \times T^t = \begin{pmatrix} 1600 & 700 \\ 700 & 1681 \end{pmatrix} = C_y$$

from which we get

$u_c(y_1) = \sqrt{} = 40 \qquad u_c(y_2) = \sqrt{} = 41$

and the correlation is

$700 / (40 * 41) = 0.427$

A non-linear relationship can (for small uncertainties) be approximated by the linear part of a Taylor's series expansion such that the transformation matrix becomes

$$\mathbf{T} = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \cdot & \cdot & \frac{\partial y_1}{\partial x_n} \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ \frac{\partial y_m}{\partial x_1} & \cdot & \cdot & \frac{\partial y_m}{\partial x_n} \end{pmatrix}_{\mathbf{x} = \langle \mathbf{x} \rangle}$$

For the elements of the covariance matrix $\mathbf{C_y}$ we get:

$$\mathrm{Cov}(y_k,y_l) \approx \sum_{i=1}^{n}\sum_{j=1}^{n} \frac{\partial y_k}{\partial x_i}\frac{\partial y_l}{\partial x_j}\mathrm{Cov}(x_i,x_j),$$

$$\mathrm{Cov}(y_k,y_k) = \mathrm{Var}(y_k) = \sigma^2(y_k)$$

The diagonal elements in $\mathbf{C_y}$ represent the variances of the output quantities, the correlations can be obtained from the off-diagonal elements. In general, $\mathbf{C_y}$ will not be diagonal (there exist nonzero off-diagonal elements) even if $\mathbf{C_x}$ is a diagonal matrix (all off-diagonal elements equal zero). The results y_k may be correlated (even if the x_i are not) because the different y_k share the same x_i.

To each element of a covariance matrix (e.g., $\mathbf{C_x}$) is associated an element of a correlation matrix (e.g., $\mathbf{Corr_x}$)

$$\mathrm{Corr}(x_i,x_j) = \frac{\mathrm{Cov}(x_i,x_j)}{\sqrt{\mathrm{Var}(x_i)}\cdot\sqrt{\mathrm{Var}(x_j)}} \approx \frac{\mathrm{Cov_e}(x_i,x_j)}{s_{x_i}\cdot s_{x_j}} \quad , \quad |\mathrm{Corr}(x_i,x_j)| \le 1$$

the diagonal elements are all equal to 1; the off-diagonal elements are zero if no correlations exist.

4. Construction of covariance matrices

If you take data from literature

- collect the actually measured quantities
- review in detail all reported corrections and their uncertainties
- verify the reported uncertainty definition, convert all to k=1 (standard uncertainty)
- note missing uncertainties
- revise reference data for recent updates

If you work on your own data

- make a list of all uncertainty components contributing in your experimental procedure
- sort for purely statistical components and components which produce correlation
- evaluate (type A or type B) standard uncertainties for all input quantities

Example 3: Preparation of uncertainty components for a series of cross sections as function of energy

Energy	E-unc.	E-res.	Data	statist.	correlated uncertainty contributions						tot.
				1	*2*	*3*		*l*		*L*	
E_1			σ_1	u_{11}	u_{12}	u_{13}		u_{1l}		u_{1L}	$u_c\sigma_1$
E_2			σ_2	u_{21}	u_{22}	u_{23}		u_{2l}		u_{2L}	$u_c\sigma_2$
E_i			σ_i	u_{i1}	u_{i2}	u_{i3}		u_{il}		u_{iL}	$u_c\sigma_i$
E_n			σ_n	u_{n1}	u_{n2}	u_{n3}		u_{nl}		u_{nL}	$u_c\sigma_n$

Construction of the covariancematrix *V*

from the table of uncertainty components

$$v_{ij} = \sum_{l=1,L}^{L} s_{ijl}\, u_{il}\, u_{jl} \qquad (i,j = 1,n)$$

$$s_{iil} = 1 \qquad 1 \geq s_{ijl} \geq -1$$

General properties of a data covariance matrix

1. A covariance matrix is by definition symmetric
2. A covariance matrix is positive (semi)definite, i.e. its eigenvalues are positive (or at least zero).

The latter is a consequence of the fact, that variances of any function of physical quantities must be non-negative and are usually not zero.

These general properties of a data covariance matrix are normally correctly produced when such a matrix is derived by including correct and complete uncertainty information into an evaluation. If due to the lack of complete information approximate methods have to be used for the assignment of covariances, special care has to be taken to guarantee that the properties pointed out above are met. Otherwise nonphysical effects will appear when processing such a covariance matrix.