Evaluation of measurement uncertainties and covariances

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Short CV

- 1988 : PhD Ghent University

  Fission fragment properties and neutron induced fission cross sections

- 1988 – 1990 : ILL Grenoble

  Nuclear structure studies (Gamma-ray spectrometry, Crystal + HPGe)

- 1990 – 2001 : JRC Ispra (I)

  Non-Destructive Analysis techniques (Nuclear Safeguards & Security)

- 2001 – : JRC Geel (B) , IRMM

  Nuclear data (Neutron induced reaction cross section measurements)

Contents

- General law of uncertainty propagation
- Propagation of correlated uncertainties
- Adjusting model parameters to experimental data (GLSQ)
- Problems related to GLSQ
- Comments on definitions and terminology

Measurement result

A quantity value being attributed to a measurand (quantity of interest) together with any other available relevant information

⇒ A measurement result includes its uncertainty

International vocabulary of metrology

Basic and general concepts and associated terms (VIM)

(JCGM 200:2012)

Evaluation of Measurement data

Guide to the expression of uncertainty in measurement

(JCGM 100 :2008)

Measurement result

Input quantities → **Output quantity (measurand)**

e.g. Determination of activity A_α based on α-spectroscopy

measured quantity : $C_\alpha = C' - B$

measurand : A_α

Model

$$C_\alpha = \varepsilon_\alpha \ \Omega \ P_\alpha \ A_\alpha$$

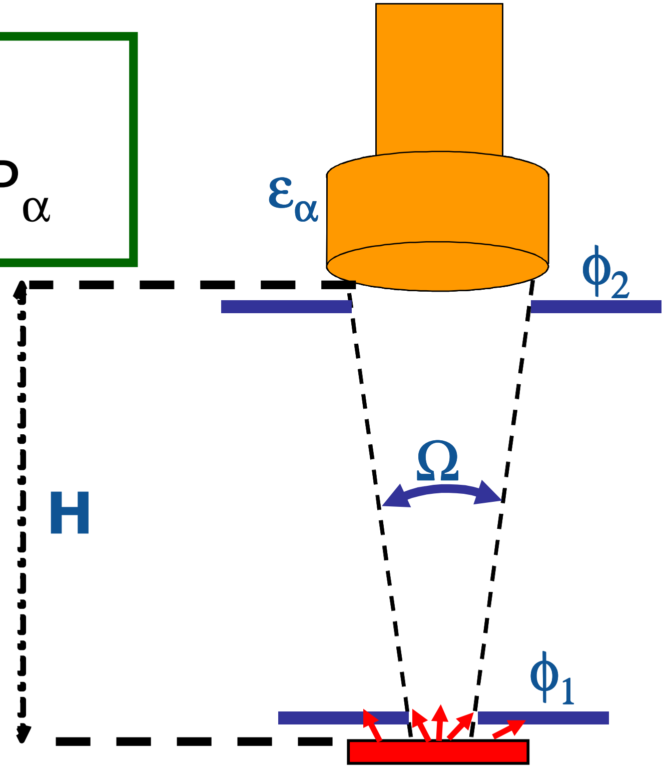
$$A_\alpha = C_\alpha \ / \ \varepsilon_\alpha \ \Omega \ P_\alpha$$

C_α : observed count rate in the peak

P_α : escape probability

Ω : solid angle depends on (H, ϕ_1, ϕ_2)

ε_α : detection efficiency



Measurement result

Input quantities → **Output quantity (measurand)**

(X_1, X_2, X_3, …) **Model** **Z**

- determination of activity A_α based on α-spectroscopy :

exp. observable : $C_\alpha = C' - B$

measurand : A_α

model : $$A_\alpha = \frac{C_\alpha}{\varepsilon_\alpha \, \Omega \, P_\alpha}$$

$$Z = \mathbf{F}(X_1, X_2, X_3, \ldots)$$

Measurement result

Input quantities → **Output quantity (measurand)**

$(X_1, X_2, X_3, \ldots)$ **Model** **Z**

- determination of activity A_α based on α-spectroscopy :

exp. observable : $C_\alpha = C' - B$

measurand : A_α

model : $A_\alpha = \frac{C_\alpha}{\varepsilon_\alpha \, \Omega \, P_\alpha}$

$Z = F(X_1, X_2, X_3, \ldots)$

- determination of decay constant

exp. observable : $C_\alpha(t)$

decay constant : λ_α

model : $C_M = e^{-\lambda_\alpha t}$

$M(Z, X_1, X_2, X_3, \ldots) = 0$

$$\chi^2(\lambda_\alpha) = (C_\alpha(t) - C_M(t))^T \, V_{C_\alpha}^{-1} \, (C_\alpha(t) - C_M(t))$$

General

Input quantities → **Output quantity (measurand)**

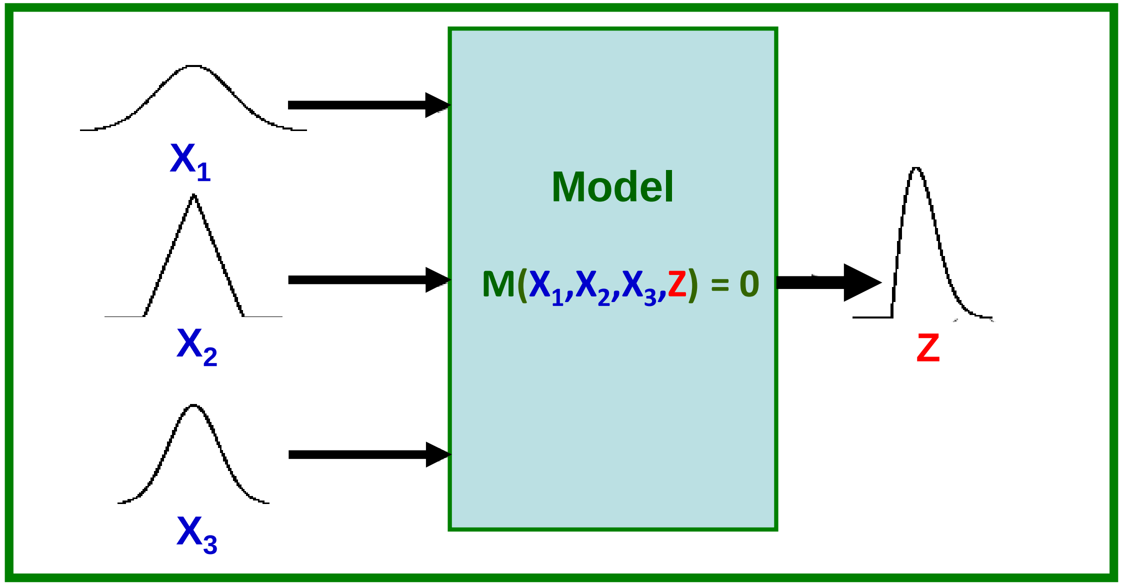
(X_1, X_2, X_3, …) **Model** **Z**

Input

- ***Measurement results***

+

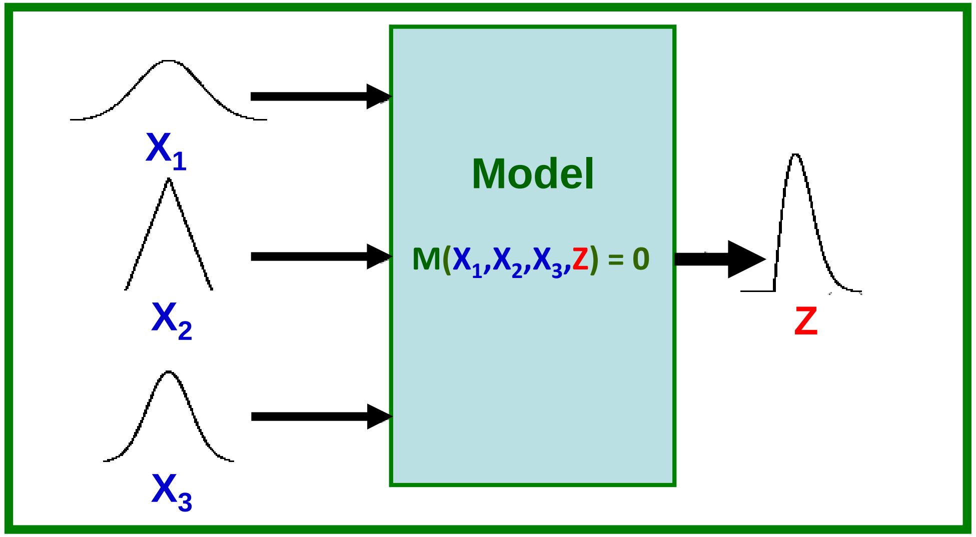
- calibration constants
- influencing quantities
- physical constants



General

Input quantities → **Output quantity (measurand)**

(X_1, X_2, X_3, …) **Model** **Z**



Ideally :

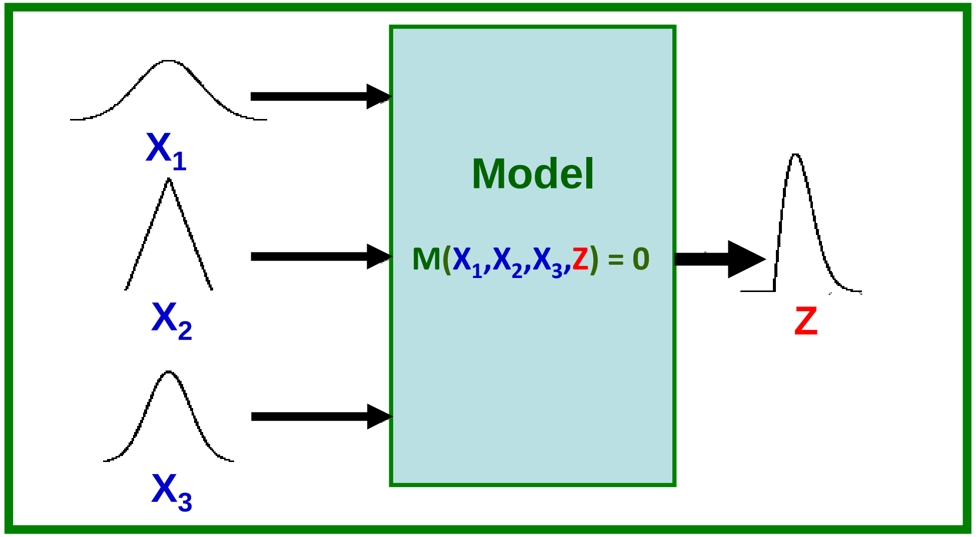
Define Probability Distribution (PD) of (X_1,X_2,X_3, …) and transform into PD of Z

- Analytically (deterministic)
- MC simulations (stochastic)

General

Input quantities → **Output quantity (measurand)**

$(X_1, X_2, X_3, \ldots)$ **Model** **Z**



Common practice :

General Law of Uncertainty Propagation (GLUP), based on:

- Properties of Normal Probability Distributions
- Combined with 1st order Taylor development for non-linear problems

Most common operations : $Z = K (Y - B)$

- **Quantity Z deduced from : $Z = Y - B$** **(B: correction)**
  - experimental observable $(y \pm u_y)$
  - application of correction (background) $(b \pm u_b)$

- **Quantity Z deduced from : $Z = K Y$** **(K : correction factor)**
  - experimental observable $(y \pm u_y)$
  - application of a correction factor $(k \pm u_k)$

GLUP : independent variables

(y,u_y), (b,u_b) and (k,u_k) independent input quantities $\Rightarrow$ estimate of Z

$$Z = Y + B \quad \Rightarrow \quad z = y + b \qquad u_z^2 = u_y^2 + u_b^2$$

$$Z = Y - B \quad \Rightarrow \quad z = y - b \qquad u_z^2 = u_y^2 + u_b^2$$

$$Z = K\,Y \quad \Rightarrow \quad z = k\,y \qquad u_z^2 = k^2\,u_y^2 + y^2 u_k^2 \qquad \frac{u_z^2}{z^2} = \frac{u_y^2}{y^2} + \frac{u_k^2}{k^2}$$

$$Z = \frac{Y}{K} \quad \Rightarrow \quad z = \frac{y}{k} \qquad u_z^2 = \frac{u_y^2}{k^2} + \frac{y^2}{k^4} u_k^2 \qquad \frac{u_z^2}{z^2} = \frac{u_y^2}{y^2} + \frac{u_k^2}{k^2}$$

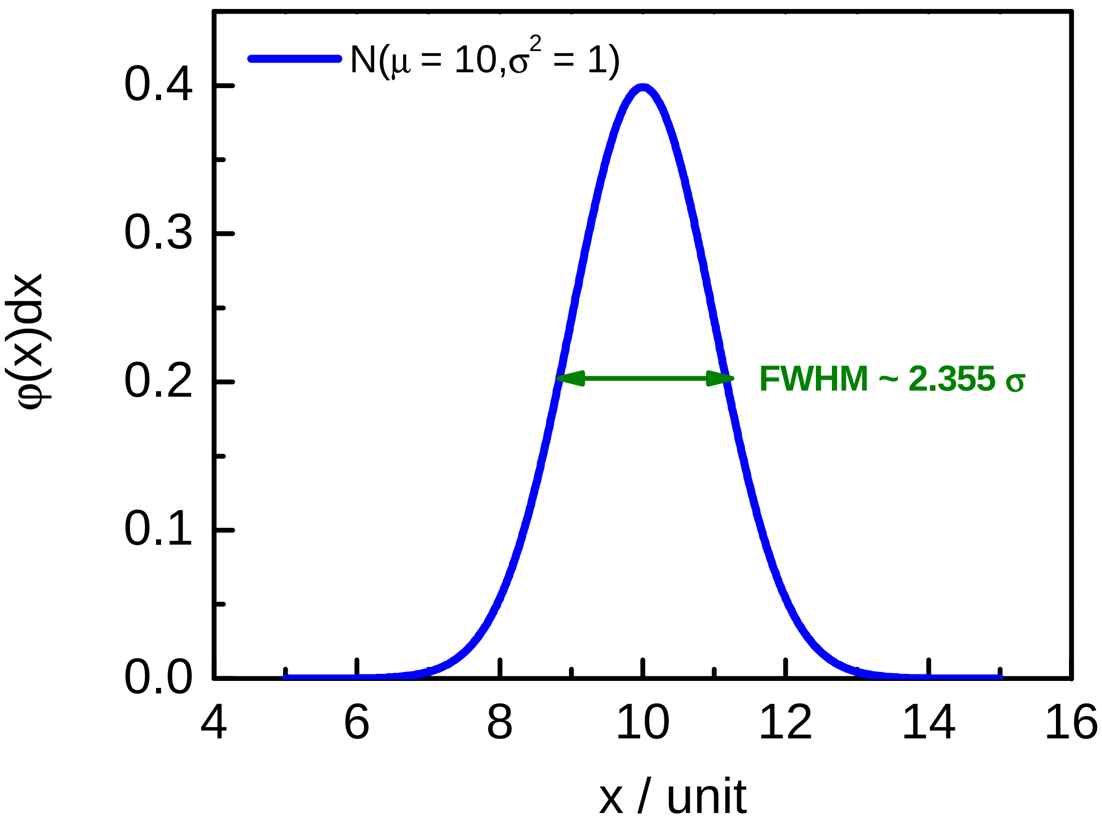
Normal (Gauss) distribution

$$\varphi(x,\mu,\sigma^2) = \frac{1}{\sqrt{2\pi}\,\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

Characteristics

- Mean : μ
- Variance : σ^2
- FWHM : $\approx 2.355\,\sigma$

Variance $\Rightarrow$ uncertainty



Linear function of independent variables

Z : linear function of independent random variables $X_{i=1,\dots,n}$ with (μ_i, σ_i^2)

PD of Z = f(X_i; i,…,n) is normal distribution with

$$Z = \sum_{i=1}^{n} c_i X_i \qquad c_i = \left.\frac{\partial f}{\partial x_i}\right|_{\mu_i}$$

- **Mean** $$\mu_Z = \sum_{i=1}^{n} c_i \mu_i$$

- **Variance** $$V(Z) = \sigma_Z^2 = \sum_{i=1}^{n} c_i^2 \sigma_i^2$$

Linear function of independent variables

Z : non-linear function of independent random variables $X_{i = 1,\ldots,n}$ with (μ_i, σ_i^2)

PD of Z = f(X_i; i,…,n) is normal distribution with

1st order Taylor development

$$Z \approx f(\mu_1,\ldots,\mu_n) + \sum_{i=1}^{n} g_i\,(x_i - \mu_i) \qquad g_i = \left.\frac{\partial f}{\partial x_i}\right|_{\mu_i}$$

- **Mean** $\mu_Z \approx f(\mu_1,\ldots,\mu_n)$
- **Variance** $V(Z) = \sigma_Z^2 \approx \sum_{i=1}^{n} g_i^2\,\sigma_i^2$

Probability distributions

(1) Poisson distribution to account for counting statistics

For large μ the distribution approaches a **normal distribution**

(2) Central limit theorem (CLT)

The sum of a large number of independent and identically-distributed random variables will be approximately **normally distributed**

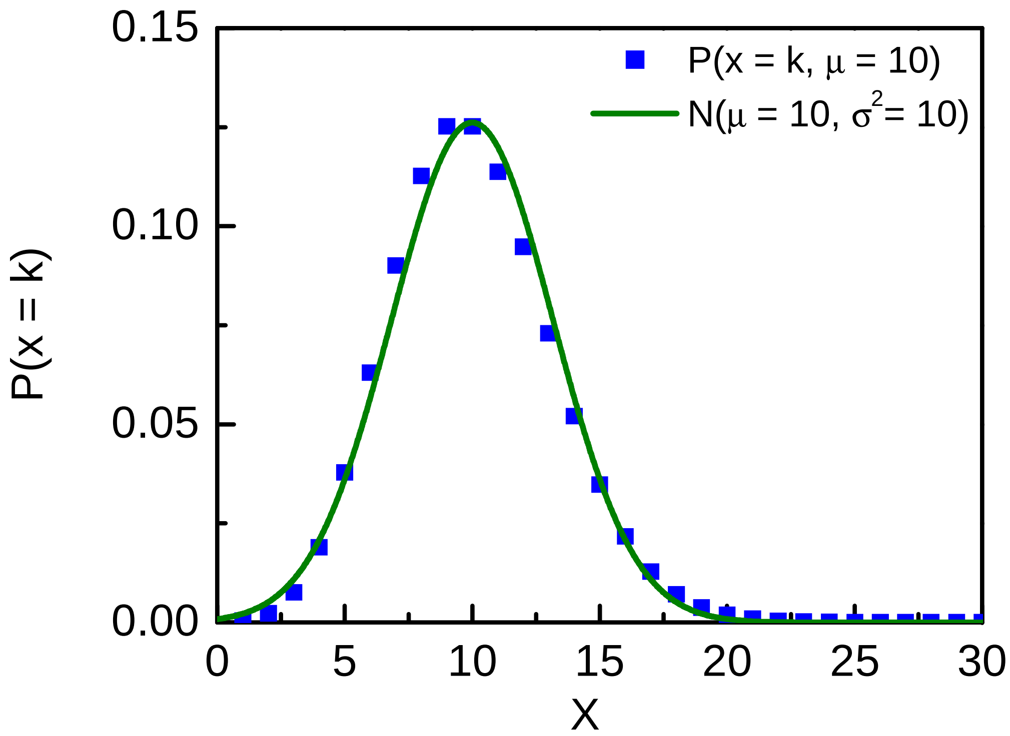
(3) Principle of maximum entropy (ME)

If only the mean and standard deviation is given, the optimal probability distribution for further inference is the **normal distribution**

$\Rightarrow$ **in most cases normal distribution can be assumed**

(1) Poisson distribution to account for counting statistics

For large μ the distribution approaches a **normal distribution**



Probability distributions

(1) Poisson distribution to account for counting statistics

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(2) Central limit theorem (CLT)

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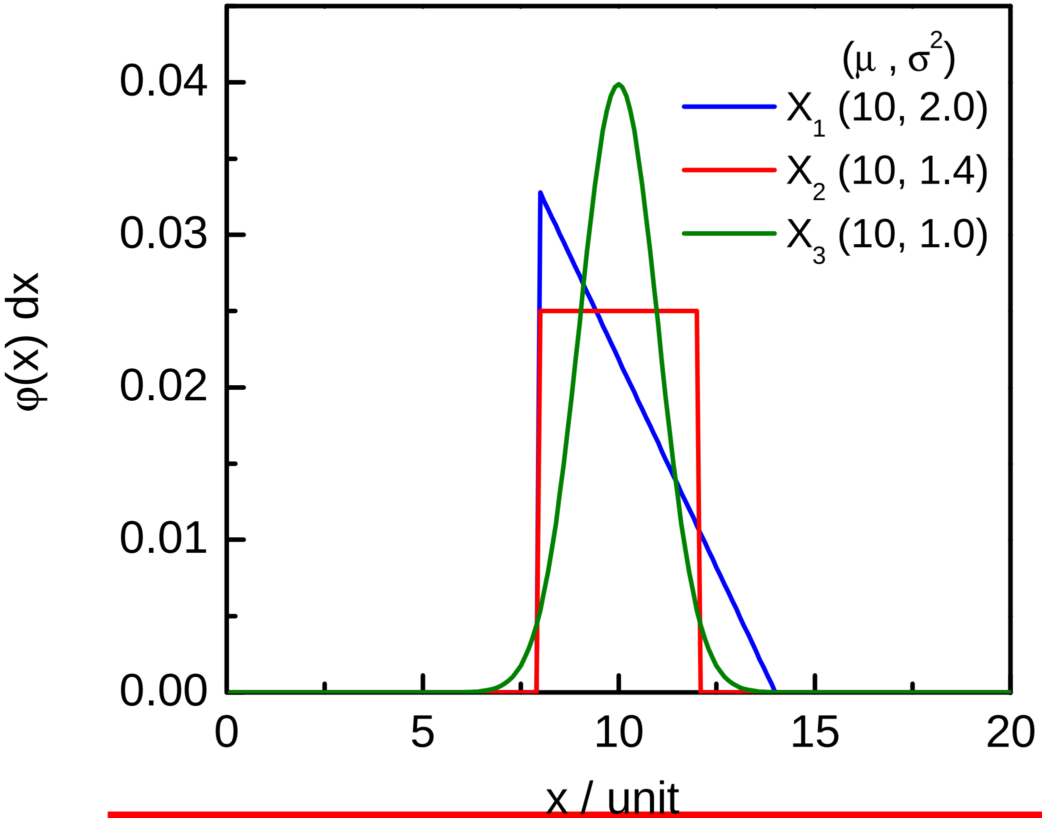
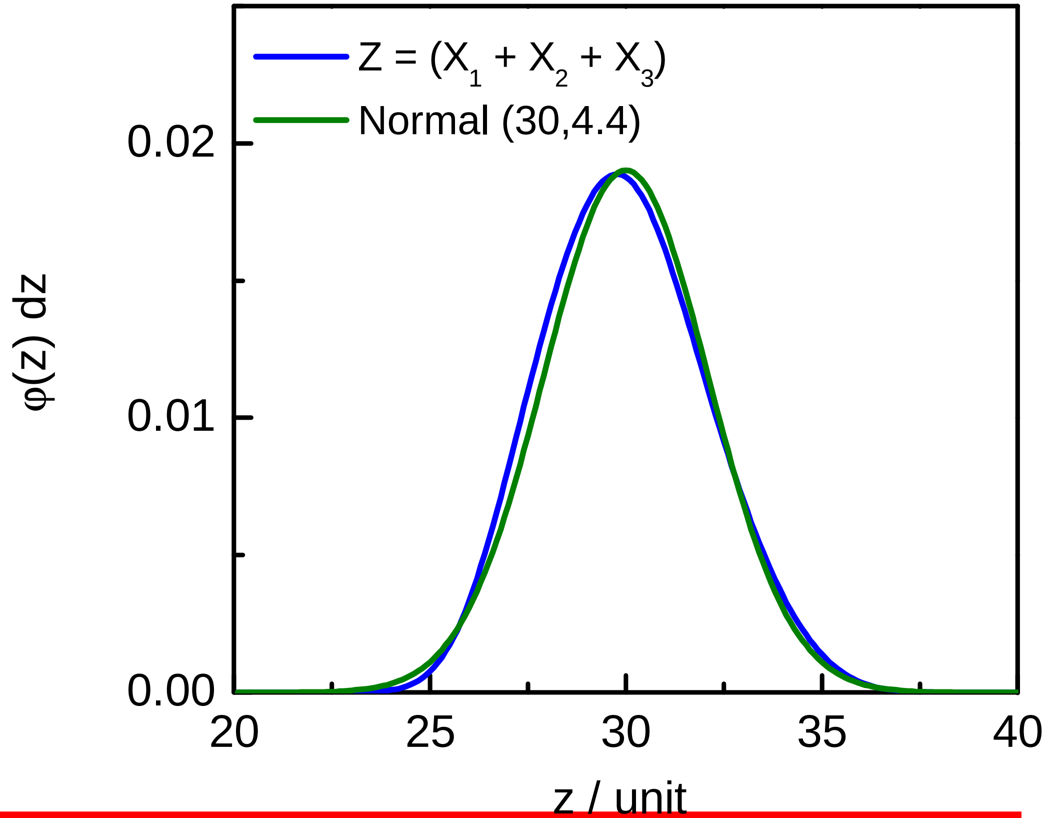
Central limit theorem





$Z = \sum_{i=1}^{n} X_i$ **normal distribution with** $\mu_Z = \sum_{i=1}^{n} \mu_i$ **and** $\sigma_Z^2 = \sum_{i=1}^{n} \sigma_i^2$

GLUP : independent variables

(y,u_y), (b,u_b) and (k,u_k) independent input quantities $\Rightarrow$ estimate of Z

$$Z = Y + B \quad \Rightarrow \quad z = y + b \qquad u_z^2 = u_y^2 + u_b^2$$

$$Z = Y - B \quad \Rightarrow \quad z = y - b \qquad u_z^2 = u_y^2 + u_b^2$$

$$Z = K\,Y \quad \Rightarrow \quad z = k\,y \qquad u_z^2 = k^2\,u_y^2 + y^2 u_k^2 \qquad \frac{u_z^2}{z^2} = \frac{u_y^2}{y^2} + \frac{u_k^2}{k^2}$$

$$Z = \frac{Y}{K} \quad \Rightarrow \quad z = \frac{y}{k} \qquad u_z^2 = \frac{u_y^2}{k^2} + \frac{y^2}{k^4} u_k^2 \qquad \frac{u_z^2}{z^2} = \frac{u_y^2}{y^2} + \frac{u_k^2}{k^2}$$

Exercise: (Y,B) ⇒ estimate of Z = Y - B

- **Experiment**

  Independent observables of Y : $(y_1 \pm u_{y_1})$ $(y_2 \pm u_{y_2})$

  Common background : $(b \pm u_b)$

- **Determine an estimate of Z = (Y- B)**

  (1) Average of (y_1, y_2) :

  (y_1,y_2) independent

$$\bar{y} = \frac{y_1 + y_2}{2} \qquad u_{\bar{y}}^2 = \frac{u_{y_1}^2 + u_{y_2}^2}{4}$$

  (2) Background subtraction :

  $(\bar{y},b)$ independent

$$\bar{z} = \bar{y} - b \qquad u_{\bar{z}}^2 = u_{\bar{y}}^2 + u_b^2$$

$$\bar{z} = \frac{y_1 + y_2}{2} - b \qquad u_{\bar{z}}^2 = \frac{u_{y_1}^2 + u_{y_2}^2}{4} + u_b^2$$

Exercise: (Y,B) ⇒ estimate of Z = Y - B

- **Experiment**

  Independent observables of Y : $(y_1 \pm u_{y_1})$ $(y_2 \pm u_{y_2})$

  Common background : $(b \pm u_b)$

- **Determine an estimate of Z = (Y- B)**

  (1) Determine of (z_1, z_2) :

$$z_1 = y_1 - b_1 \qquad u_{z_1}^2 = u_{y_1}^2 + u_b^2$$

$$z_2 = y_2 - b_2 \qquad u_{z_2}^2 = u_{y_2}^2 + u_b^2$$

  (2) Average of (z_1, z_2) :

  <u>suppose</u> (z_1,z_2) independent

$$\bar{z} = \frac{z_1 + z_2}{2} \qquad u_{\bar{z}}^2 = \frac{u_{z_1}^2 + u_{z_2}^2}{4}$$

$$\bar{z} = \frac{y_1 + y_2}{2} - b \qquad u_{\bar{z}}^2 = \frac{u_{y_1}^2 + u_{y_2}^2}{4} + \frac{u_b^2}{2}$$

Exercise: (Y,B) ⇒ estimate of Z = Y - B

Experimental data (y_1,y_2) and b : independent

(1) Subtract b from $\bar{y}$ (full details of the experiment are required) :

$$\bar{z} = \frac{y_1 + y_2}{2} - b \qquad u_{\bar{z}}^2 = \frac{u_{y_1}^2 + u_{y_2}^2}{4} + u_b^2$$

(2) Based on reporting of only (z_1,u_{z_1}) and (z_2, u_{z_2}) (*supposing* that (z_1, z_2) are independent)

$$\bar{z} = \frac{z_1 + z_2}{2} = \frac{y_1 + y_2}{2} - b \qquad u_{\bar{z}}^2 = \frac{u_{z_1}^2 + u_{z_2}^2}{4} \qquad u_{\bar{z}}^2 = \frac{u_{y_1}^2 + u_{y_2}^2}{4} + \frac{u_b^2}{2}$$

(z_1, z_2) are not independent !

Linear function of variables (normal PDF)

Z : linear function of random variables $X_{i=1,\ldots,n}$ with $(\mu_i = 1,\ldots,n; \underline{V}_{\vec{X}})$

$$Z = f(X_i;\ i = 1,\ldots,n) \qquad Z = \sum_{i=1}^{n} c_i X_i \qquad c_i = \left.\frac{\partial f}{\partial x_i}\right|_{\mu_i}$$

	Mean	**Variance**
▪ Independent variables :	$\mu_Z = \sum_{i=1}^{n} c_i \mu_i$	$\sigma_Z^2 = \sum_{i=1}^{n} c_i^2 \sigma_i^2$
▪ Dependent variables:	$\mu_Z = \sum_{i=1}^{n} c_i \mu_i$	$\sigma_Z^2 = \sum_{i=1}^{n} c_i^2 \sigma_i^2 + \sum_{i \neq} \sum_{j} c_i c_j v_{ij}$

GLUP : linear function, Z vector dim. m

$$\vec{Z} = \underline{C}\,\vec{X} \qquad \underline{V}_{\vec{Z}} = \underline{C}\,\underline{V}_{\vec{X}}\,\underline{C}^T \qquad c_{ik} = \frac{\partial f_i}{\partial x_k}$$

$$\underline{V}_{\vec{Z}} = \begin{bmatrix} c_{11} & c_{12} & . & . & . & c_{1n} \\ c_{21} & c_{22} & . & . & . & c_{2n} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ c_{m1} & c_{m2} & . & . & . & c_{mn} \end{bmatrix} \begin{bmatrix} \sigma_1^2 & v_{12} & . & . & . & v_{1n} \\ v_{21} & \sigma_2^2 & . & . & . & v_{2n} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ v_{n1} & v_{n2} & . & . & . & \sigma_n^2 \end{bmatrix} \begin{bmatrix} c_{11} & c_{21} & . & . & . & c_{m1} \\ c_{12} & c_{22} & . & . & . & c_{m2} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ c_{1n} & c_{2n} & . & . & . & c_{mn} \end{bmatrix}$$

General Law of Uncertainty Propagation (GLUP)

GLUP : (Y,B) ⇒ estimate of Z = Y - B

$$(y_1, u_{y_1}), (y_2, u_{y_2}) \text{ and } (b, u_b) \xrightarrow{(1)} (z_1, z_2) = (y_1 - b, y_2 - b) \text{ and } V_{z_1,z_2} \xrightarrow{(2)} (\bar{z}, u_{\bar{z}})$$

(y_1, y_2, b) : independent

(1) Determine $(z_1,z_2) = (y_1\text{-}b,\ y_2\text{-}b)$ and V_{z_1,z_2} from (y_1,u_{y_1}), (y_2,u_{y_2}) and (b,u_b)

(2) Determine $(\bar{z}, u_{\bar{z}})$ from (z_1,z_2) and V_{z_1,z_2}

GLUP : (Y,B) ⇒ estimate of Z = Y - B

$$(y_1, u_{y_1}), (y_2, u_{y_2}) \text{ and } (b, u_b) \quad \xrightarrow{(1)} \quad (z_1, z_2) = (y_1 - b, y_2 - b) \text{ and } \underline{V}_{z_1,z_2} = \underline{C}\,\underline{V}_{y_1,y_2,b}\,\underline{C}^T$$

(y_1,y_2,b) : independent

Step (1)

1) Determine $\underline{V}_{y_1,y_2,b}$

independent observables
⇒ uncorrelated uncertainties

$$\underline{V}_{y_1,y_2,b} = \begin{bmatrix} u_{y_1}^2 & 0 & 0 \\ 0 & u_{y_2}^2 & 0 \\ 0 & 0 & u_b^2 \end{bmatrix}$$

2) Determine $\underline{C}$

model : Z = Y - B

$$\underline{C} = \begin{bmatrix} \frac{\partial Z_1}{\partial Y_1} & \frac{\partial Z_1}{\partial Y_2} & \frac{\partial Z_1}{\partial B} \\ \frac{\partial Z_2}{\partial Y_1} & \frac{\partial Z_2}{\partial Y_2} & \frac{\partial Z_2}{\partial B} \end{bmatrix} = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \end{bmatrix}$$

3) $\underline{V}_{\vec{z}} = \underline{C}\,\underline{V}_{y_1,y_2,b}\,\underline{C}^T$

GLUP : (Y,B) ⇒ estimate of Z = Y - B

$$(y_1, u_{y_1}), (y_2, u_{y_2}) \text{ and } (b, u_b) \;\rightarrow\; (z_1, z_2) = (y_1 - b, y_2 - b) \text{ and } \underline{V}_{z_1,z_2} = \underline{C}\,\underline{V}_{y_1,y_2,b}\,\underline{C}^T$$

(y_1, y_2, b) : independent (1)

Step (1)

$$\underline{V}_{\vec{z}} = \underline{C}\,\underline{V}_{y_1,y_2,b}\,\underline{C}^T$$

$$\underline{V}_{z_1,z_2} = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} u_{y_1}^2 & 0 & 0 \\ 0 & u_{y_2}^2 & 0 \\ 0 & 0 & u_b^2 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ -1 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} u_{y_1}^2 & 0 \\ 0 & u_{y_2}^2 \\ -u_b^2 & -u_b^2 \end{bmatrix}$$

$$\underline{V}_{z_1,z_2} = \begin{bmatrix} u_{y_1}^2 + u_b^2 & u_b^2 \\ u_b^2 & u_{y_2}^2 + u_b^2 \end{bmatrix}$$

GLUP : (Y,B) ⇒ estimate of Z = Y - B

$$(y_1, u_{y_1}), (y_2, u_{y_2}) \text{ and } (b, u_b) \xrightarrow{(1)} (z_1, z_2) = (y_1 - b, y_2 - b) \text{ and } V_{z_1,z_2} \xrightarrow{(2)} (\bar{z}, u_{\bar{z}})$$

(y_1, y_2, b) : independent

Step (1) : Determine $(z_1,z_2) = (y_1\text{-}b,\ y_2\text{-}b)$ and covariance matrix V_{z_1,z_2}

$$(z_1, z_2) \qquad \underline{V}_{\vec{z}} = \underline{C}\,\underline{V}_{y_1,y_2,b}\,\underline{C}^T \qquad \underline{V}_{z_1,z_2} = \begin{bmatrix} u_{y_1}^2 + u_b^2 & u_b^2 \\ u_b^2 & u_{y_2}^2 + u_b^2 \end{bmatrix}$$

Step (2) : Determine ($\bar{z}$, $u_{\bar{z}}$)

$$\bar{z} = \frac{z_1 + z_2}{2} \qquad V_{\bar{z}} = \underline{C}\,\underline{V}_{z_1,z_2}\,\underline{C}^T$$

$$\underline{C} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \end{bmatrix} \qquad \underline{V}_{\bar{z}} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \end{bmatrix} \begin{bmatrix} u_{y_1}^2 + u_B^2 & u_b^2 \\ u_b^2 & u_{y_2}^2 + u_b^2 \end{bmatrix} \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix} = \frac{u_{y_1}^2 + u_{y_2}^2}{4} + u_b^2$$

GLUP : (Y,B) ⇒ estimate of Z = Y - B

Experimental data (y_1,y_2) and b : independent

(1) With full details about experiment: first average of (y_1,y_2)

$$\bar{z} = \frac{y_1 + y_2}{2} - b$$

$$u_{\bar{z}}^2 = \frac{u_{y_1}^2 + u_{y_2}^2}{4} + u_b^2$$

(2) Based on reporting of (z_1, z_2) and $\underline{V}_{z_1,z_2}$

$$\bar{z} = \frac{y_1 + y_2}{2} - b$$

Full covariance

$$u_{\bar{z}}^2 = \frac{u_{y_1}^2 + u_{y_2}^2}{4} + u_b^2$$

Only diagonal terms

$$u_{\bar{z}}^2 = \frac{u_{y_1}^2 + u_{y_2}^2}{4} + \frac{u_b^2}{2}$$

Linear function of variables (normal PDF)

Z : linear function of random variables $X_{i = 1,\ldots,n}$ with $(\mu_i = 1,\ldots,n; \underline{V}_{\vec{X}})$

$$Z = f(X_i;\ i = 1,\ldots,n) \qquad Z = \sum_{i=1}^{n} c_i\, X_i \qquad c_i = \left.\frac{\partial f}{\partial x_i}\right|_{\mu_i}$$

	Mean	**Variance**
▪ Independent variables :	$\mu_Z = \sum_{i=1}^{n} c_i\, \mu_i$	$\sigma_Z^2 = \sum_{i=1}^{n} c_i^2\, \sigma_i^2$
▪ Dependent variables:	$\mu_Z = \sum_{i=1}^{n} c_i\, \mu_i$	$\sigma_Z^2 = \sum_{i=1}^{n} c_i^2\, \sigma_i^2 + \boxed{\sum_{i \neq} \sum_{j} c_i\, c_j\, v_{ij}}$

Linear function of variables (normal PDF)

Z : non-linear function of random variables $X_{i=1,\ldots,n}$ with $(\mu_i = 1,\ldots,n; \underline{V}_{\vec{X}})$

$$Z = f(X_i;\ i = 1,\ldots,n) \qquad Z \approx f(\mu_1,\ldots,\mu_n) + \sum_{i=1}^{n} g_i\,(x_i - \mu_i) \qquad g_i = \left.\frac{\partial f}{\partial x_i}\right|_{\mu_i}$$

1st order Taylor development

Mean **Variance**

- Independent variables : $\mu_Z \approx f(\mu_1,\ldots,\mu_n)$ $\quad \sigma_Z^2 \approx \sum_{i=1}^{n} g_i^2\,\sigma_i^2$
- Dependent variables: $\mu_Z \approx f(\mu_1,\ldots,\mu_n)$ $\quad \sigma_Z^2 \approx \sum_{i=1}^{n} g_i^2\,\sigma_i^2 + \sum_{i\neq}\sum_{j} g_i\,g_j\,v_{ij}$

	Linear	**Non - linear**
$\vec{Z} = \vec{f}(X_i;\ i = 1,\ldots,n)$	$\vec{Z} = \underline{C}\,\vec{X}$	$\vec{Z} \approx \vec{f}(\vec{\mu}_X) + \underline{G}_{\vec{X}}(\vec{x} - \vec{\mu}_X)$
	$\underline{C}$: dim (m x n)	$\underline{G}_X$: sensitivity matrix dim (m x n)
	$c_{ik} = \dfrac{\partial f_i}{\partial x_k}$	$g_{ik} = \dfrac{\partial f_i}{\partial x_k}$
• **Mean**	$\vec{\mu}_z = \underline{C}\ \vec{\mu}_X$	$\vec{\mu}_z \approx \vec{f}(\vec{\mu}_x)$
• **Covariance matrix**	$\underline{V}_{\vec{Z}} = \underline{C}\ \underline{V}_{\vec{X}}\ \underline{C}^T$	$\underline{V}_Z \approx \underline{G}_X\ \underline{V}_X\ \underline{G}_X^T$

⇒ basis of General Law of Uncertainty Propagation (GLUP)
(sandwich formula, $V_z = G\ V_x\ G^T$)

GLUP : (Y,B) $\Rightarrow$ Z = Y - B

$$(y_1, u_{y_1}), (y_2, u_{y_2}), \ldots, (y_n, u_{y_n}) \text{ and } (b, u_b) \rightarrow (z_1, u_{y_1}), (z_2, u_{z_2}), \ldots, (z_n, u_{z_n})$$

$(y_1, y_2, \ldots, y_n, b)$: independent $\qquad z_i = y_i - b$

$(z_1, z_2, \ldots, z_n) = (y_1 - b), (y_2 - b), \ldots, (y_n - b)$

$$\underline{V}_{\vec{z}} = \begin{bmatrix} u_{y_1}^2 + u_b^2 & u_b^2 & \cdot & \cdot & \cdot & u_b^2 \\ u_b^2 & u_{y_2}^2 + u_b^2 & \cdot & \cdot & \cdot & u_b^2 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ u_b^2 & u_b^2 & \cdot & \cdot & \cdot & u_{y_n}^2 + u_b^2 \end{bmatrix}$$

GLUP : (Y,B) $\Rightarrow$ estimate of Z = Y - B

$$(y_1, u_{y_1});(y_2, u_{y_2}),\ldots,(y_n, u_{y_n}) \text{ and } (b, u_b) \rightarrow (\bar{z}, u_{\bar{z}})$$

$(y_1, y_2, \ldots, y_n, b)$: independent

$$\bar{z} = \frac{1}{m}\sum_{j=1}^{m} y_j - b \qquad u_{\bar{z}}^2 = \frac{1}{m^2}\sum_{j=1}^{m} u_{y_j}^2 + u_b^2$$

$$\bar{z} = \bar{y} - b \qquad u_{\bar{z}} = \sqrt{\frac{1}{m^2}\sum_{j=1}^{n} u_{y_j}^2 + u_b^2}$$

GLUP : (Y,K) $\Rightarrow$ Z = KY

$$(y_1, u_{y_1}), (y_2, u_{y_2}), \ldots, (y_n, u_{y_n}) \text{ and } k, u_k) \quad \rightarrow \quad (z_1, u_{y_1}), (z_2, u_{z_2}), \ldots, (z_n, u_{z_n})$$

$(y_1, y_2, \ldots, y_n, b)$: independent $\qquad z_i = k\, y_i$

$(z_1, z_2, \ldots, z_n) = (ky_1 , ky_2 , \ldots, ky_n)$

$$\underline{V}_{\vec{z}} = \begin{bmatrix} k^2 u_{y_1}^2 + y_1^2 u_k^2 & y_1 y_2 u_k^2 & \cdot & \cdot & \cdot & y_1 y_n u_k^2 \\ y_2 y_1 u_k^2 & k^2 u_{y_2}^2 + y_2^2 u_k^2 & \cdot & \cdot & \cdot & y_2 y_n u_{Kk}^2 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & k^2 u_{y_{n-1}}^2 & y_{n-1} y_n u_k^2 \\ y_n y_1 u_k^2 & y_n y_2 u_k^2 & \cdot & \cdot & y_n y_{n-1} u_k^2 & k^2 u_{y_n}^2 + y_n^2 u_k^2 \end{bmatrix}$$

GLUP : (Y,B) $\Rightarrow$ estimate of Z = KY

$$(y_1, u_{y_1});(y_2, u_{y_2}),\dots,(y_n, u_{y_n}) \text{ and } (k, u_k) \rightarrow (\bar{z}, u_{\bar{z}})$$

$(y_1, y_2, \dots, y_n, b)$: independent

$$\bar{z} = k\frac{1}{m}\sum_{j=1}^{m} y_j \qquad u_{\bar{z}}^2 = \frac{k^2}{m^2}\sum_{j=1}^{m} u_{y_j}^2 + \bar{y}^2 u_k^2$$

$$\bar{z} = k\,\bar{y} \qquad u_{\bar{z}} = \sqrt{\frac{k^2}{m^2}\sum_{j=1}^{m} u_{y_j}^2 + \bar{y}^2 u_k^2}$$

Covariance and correlation matrix

$$(z_1, z_2) = (y_1 - b, y_2 - b)$$

Covariance matrix

- **Symmetric**
- **Positive definite (see AGS presentation)**

$$\underline{V}_{z_1,z_2} = \begin{bmatrix} u_{y_1}^2 + u_b^2 & u_b^2 \\ u_b^2 & u_{y_2}^2 + u_b^2 \end{bmatrix}$$

$$\underline{\rho}_{z_1,z_2} = \begin{bmatrix} 1 & \dfrac{u_b^2}{\sqrt{(u_{y_1}^2 + u_b^2)(u_{y_2}^2 + u_b^2)}} \\ \dfrac{u_b^2}{\sqrt{(u_{y_1}^2 + u_b^2)(u_{y_2}^2 + u_b^2)}} & 1 \end{bmatrix}$$

$$\rho(z_1, z_2) = \frac{u_b^2}{\sqrt{(u_{y_1}^2 + u_b^2)(u_{y_2}^2 + u_b^2)}}$$

Adjustment of model parameters to exp. data

Problem: n data points (x_1,y_1), …, (x_n, y_n) and a model $\vec{Y} = f(\vec{X},\vec{p})$

Y depends on X and parameters $(p_1,\ldots,p_k)$ with n>k.

Determine from the experimental data $(\vec{x}, \vec{y})$ the best estimate of parameters $(p_1,\ldots,p_k)$

Background model

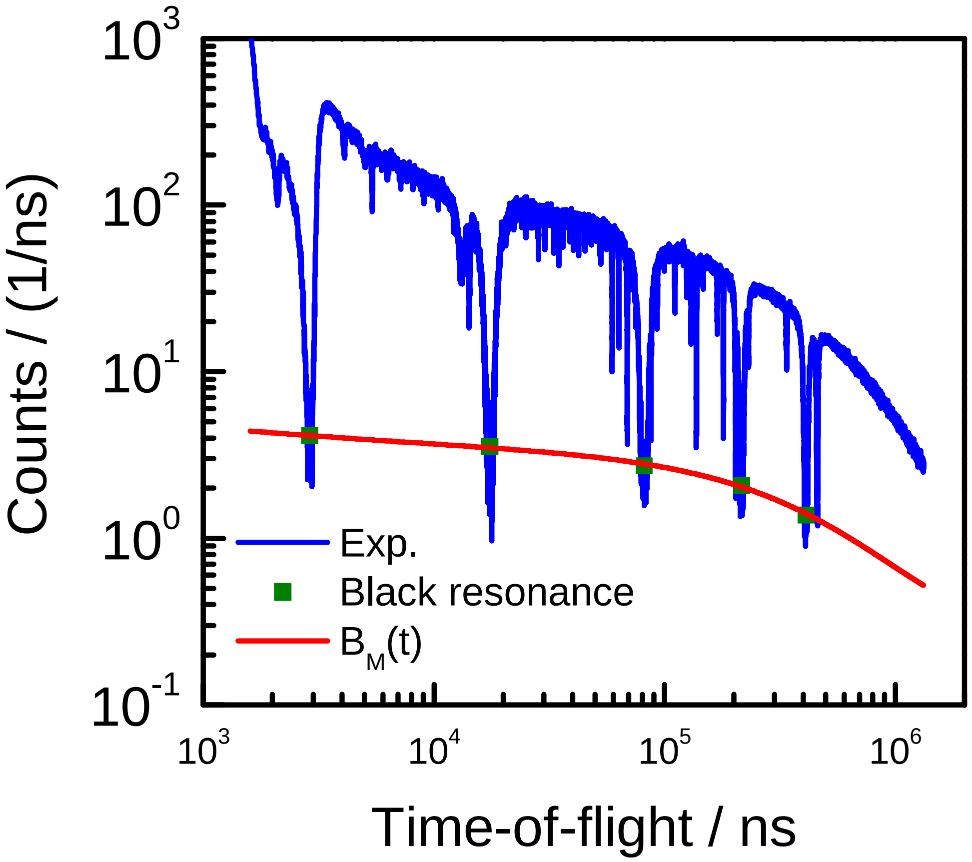
$$B_M(t) = b_0 + b_1\, e^{-\lambda_1 t} + b_2\, e^{-\lambda_2 t} + b_3\, e^{-\lambda_3 (t+t_0)}$$

Determine best estimate of:

$$\vec{p} = (b_0, b_1, \lambda_1, b_2, \lambda_2, b_3, \lambda_3)$$

by minimizing

$$\chi^2(\vec{p}) = (B_{exp}(t) - B_M(t,\vec{p}))^T\, \underline{V}_{B_{exp}}^{-1}\, (B_{exp}(t) - B_M(t,\vec{p}))$$



Adjustment of model parameters to exp. data

Z_{exp} : experimental observable

$Z_M(t,\eta,\kappa)$: model for theoretical estimate of Z_{exp}

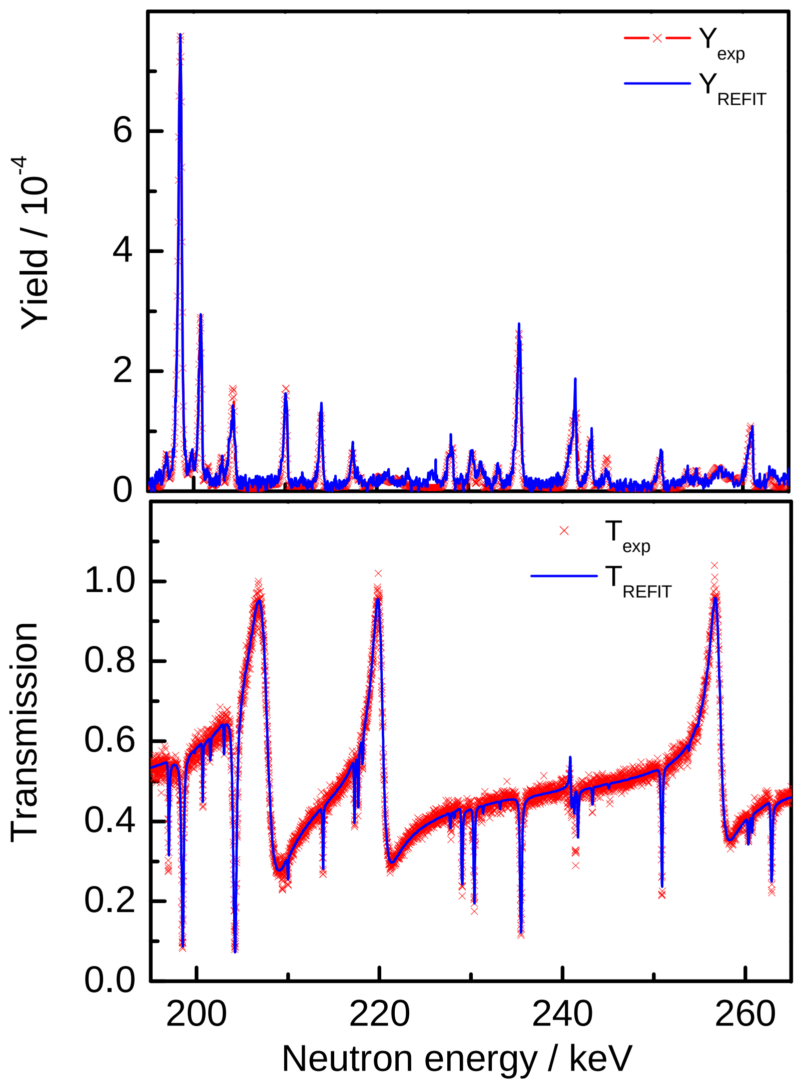
Model:

- R-matrix theory : parameterisation of σ by RP (η)
- Experiment : parameter vector κ

$$Z_M(E) = \begin{cases} T(E) = e^{-n\bar{\sigma}_{tot}} \\ Y_r(E) = (1 - e^{-n\bar{\sigma}_{tot}}) \dfrac{\bar{\sigma}_r}{\bar{\sigma}_{tot}} + \ldots \end{cases}$$

$$Z_M(t) = \frac{\int R(t,E)\; Z_M(E)dE}{\int R(t,E)dE} \quad \longleftrightarrow \quad Z_{exp}(t)$$

$^{206}Pb + n$



Least Squares Adjustment (LSQ)

$$\vec{Y}_M = \underline{G}_{\vec{p}}\,\vec{p}$$

$$(x_1,y_1),\ (x_2,y_2),\ (x_3,y_3)\quad +\quad V_{\vec{y}}$$

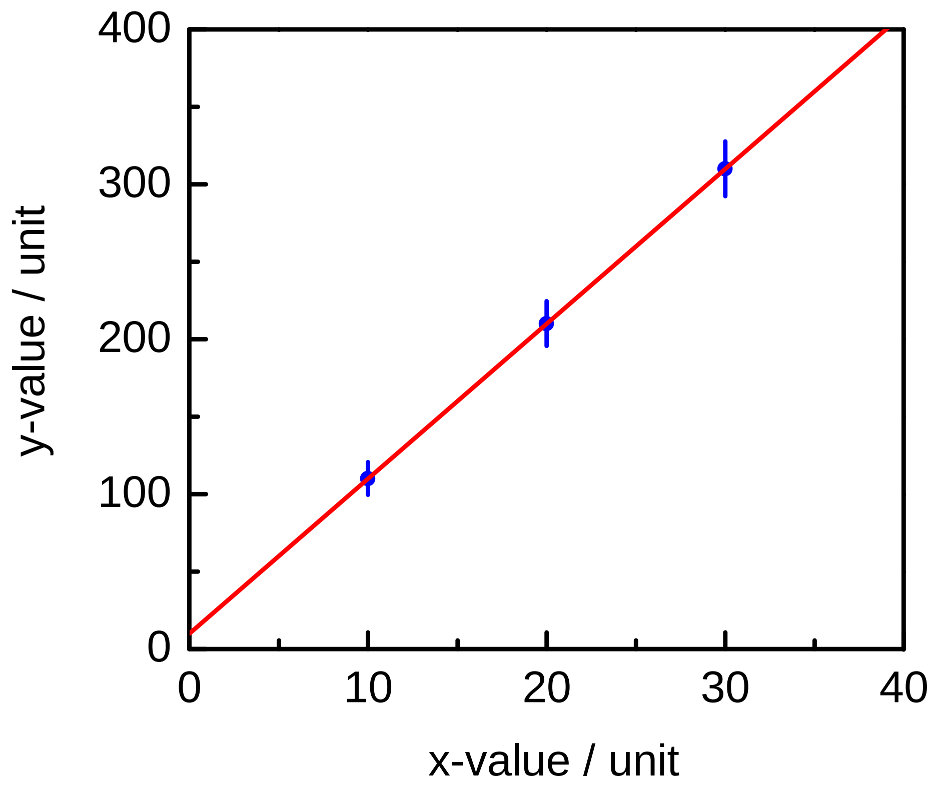
$$\vec{Y}_M = a_0 + a_1 \vec{X}$$

$$\chi^2(\vec{p})_{min} = (\vec{y} - f_M(\vec{x},\vec{p}))^T\,\underline{V}_{\vec{y}}^{-1}\,(\vec{y} - f_M(\vec{x},\vec{p}))$$

$$\vec{p} = (a_0, a_1)$$

$$\vec{p} = V_{\vec{p}}\,\underline{G}_{\vec{p}}^T\,\underline{V}_{\vec{y}}^{-1}\,\vec{y}$$

$$\underline{V}_p = (\underline{G}_{\vec{p}}^T\,\underline{V}_{\vec{y}}^{-1}\,\underline{G}_{\vec{p}})^{-1}$$



Least Squares Adjustment (LSQ)

$$\vec{Y}_M = \underline{G}_{\vec{p}}\,\vec{p}$$

$$(x_1,y_1),\ (x_2,y_2),\ (x_3,y_3)\ +\ V_{\vec{y}}$$

$$\vec{Y}_M = a_0 + a_1\vec{X}$$

$$\chi^2(\vec{p})_{min} = (\vec{y} - f_M(\vec{x},\vec{p}))^T\,\underline{V}_{\vec{y}}^{-1}\,(\vec{y} - f_M(\vec{x},\vec{p}))$$

$$\vec{p} = (a_0, a_1)$$

$$\vec{p} = V_{\vec{p}}\,\underline{G}_{\vec{p}}^T\,\underline{V}_{\vec{y}}^{-1}\,\vec{y}$$

$$\underline{V}_p = (\underline{G}_{\vec{p}}^T\,\underline{V}_{\vec{y}}^{-1}\,\underline{G}_{\vec{p}})^{-1}$$

Input from experiment

$$\vec{y} = (y_1, y_2, y_3)$$

$$\underline{V}_{\vec{y}} = \begin{bmatrix} u_{y_1}^2 & 0 & 0 \\ 0 & u_{y_2}^2 & 0 \\ 0 & 0 & u_{y_3}^2 \end{bmatrix}$$

Model

$$\underline{G}_{\vec{p}} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \end{bmatrix}$$

Least Squares Adjustment (LSQ)

Problem: $\vec{Y} = f(\vec{X}, \vec{p})$ depends on X and parameter vector $(p_1,\ldots,p_k)$

n experimental data points $(x_1,y_1), \ldots, (x_n, y_n)$ with covariance $\underline{V}_{\vec{y}}$

Determine from the data $(\vec{x}, \vec{y})$ the best estimate of $(p_1,\ldots,p_k)$ $(n > k)$.

(1) Maximum likelihood : vector $\vec{p}$ which maximizes the likelihood

$$\Rightarrow \text{maximize:} \quad L\left((\vec{y}, \underline{V}_{\vec{y}}) \middle| \vec{p}\right) = \frac{1}{\sqrt{\det(2\pi \underline{V}_{\vec{y}})}} e^{-\frac{1}{2}(\vec{y}-f(\vec{x},\vec{p}))^T \underline{V}_{\vec{y}}^{-1} (\vec{z}-f(\vec{x},\vec{p}))}$$

$$\Rightarrow \text{minimize:} \quad \chi^2(\vec{p}) = (\vec{y} - f(\vec{x},\vec{p}))^T \underline{V}_{\vec{y}}^{-1} (\vec{y} - f(\vec{x},\vec{p}))$$

(2) Least squares adjustment : vector $\vec{p}$ which minimizes the expression

$$\Rightarrow \text{minimize:} \quad \chi^2(\vec{p}) = (\vec{y} - f(\vec{x},\vec{p}))^T \underline{V}_{\vec{y}}^{-1} (\vec{y} - f(\vec{x},\vec{p}))$$

Least Squares Adjustment (LSQ)

Problem: $\vec{Y} = f(\vec{X}, \vec{p})$ depends on X and parameter vector $(p_1,\ldots,p_k)$

n experimental data points $(x_1,y_1), \ldots, (x_n, y_n)$ with covariance $\underline{V}_{\vec{y}}$

Determine from the data $(\vec{x}, \vec{y})$ the best estimate of $(p_1,\ldots,p_k)$ $(n > k)$.

(1) Maximum likelihood : vector $\vec{p}$ which maximizes the likelihood

$$\Rightarrow \text{maximize:} \quad L\left((\vec{y}, \underline{V}_{\vec{y}}) \middle| \vec{p}\right) = \frac{1}{\sqrt{\det(2\pi \underline{V}_{\vec{y}})}} e^{-\frac{1}{2}(\vec{y}-f(\vec{x},\vec{p}))^T \underline{V}_{\vec{y}}^{-1} (\vec{z}-f(\vec{x},\vec{p}))}$$

$$\Rightarrow \text{minimize:} \quad \chi^2(\vec{p}) = (\vec{y} - f(\vec{x},\vec{p}))^T \, \underline{V}_{\vec{y}}^{-1} \, (\vec{y} - f(\vec{x},\vec{p}))$$

Least squares adjustment (LSQ)

(2) Least squares adjustment : vector $\vec{p}$ which *minimizes a sum of squares*

$$\Rightarrow \text{minimize:} \quad \chi^2(\vec{p}) = \sum_{i=1}^{n} \frac{1}{u_{y_i}^2} (y_i - f(x_i, \vec{p}))^2$$

for independent data points $(x_1,y_1), \ldots, (x_n, y_n)$

LSQ : linear model (example)

Input from experiment : $(\vec{x}, \vec{y})$ $\quad V_{\vec{y}}$

Model : $\vec{Y} = f(\vec{X}, \vec{p})$

Minimize : $\chi^2(\vec{p}) = (\vec{y} - f(\vec{x}, \vec{p}))^T \underline{V}_{\vec{y}}^{-1} (\vec{y} - f(\vec{x}, \vec{p}))$

Linear model

$$\vec{Y} = \underline{G}_{\vec{p}} \, \vec{p} \qquad g_{p,ij} = \frac{\partial f_i}{\partial p_j}$$

$$\vec{p} = V_{\vec{p}} \, \underline{G}_{\vec{p}}^T \, \underline{V}_{\vec{y}}^{-1} \, \vec{y}$$

$$\underline{V}_p = (\underline{G}_{\vec{p}}^T \, \underline{V}_{\vec{y}}^{-1} \, \underline{G}_{\vec{p}})^{-1}$$

$$\vec{Y} = \sum_{j=0}^{k} a_j \, \vec{X}^j \qquad \vec{p} = (a_o, \ldots, a_k)$$

$$\underline{G}_{\vec{p}} = \begin{bmatrix} 1 & x_1 & . & . & . & x_1^k \\ 1 & x_2 & . & . & . & x_2^k \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ 1 & x_n & . & . & . & x_n^k \end{bmatrix}$$

LSQ : non-linear model

Input from experiment : $(\vec{x}, \vec{y})$ $\quad V_{\vec{y}}$

Model : $\vec{Y} = f(\vec{X}, \vec{p})$

Minimize : $\chi^2(\vec{p}) = (\vec{y} - f(\vec{x}, \vec{p}))^T \underline{V}_{\vec{y}}^{-1} (\vec{y} - f(\vec{x}, \vec{p}))$

Linear model

$$\vec{Y} = \underline{G}_{\vec{p}} \vec{p}$$

$$g_{p,ij} = \frac{\partial f_i}{\partial p_j}$$

$$\vec{p} = V_{\vec{p}} \underline{G}_{\vec{p}}^T \underline{V}_{\vec{y}}^{-1} \vec{y}$$

$$\underline{V}_p = (\underline{G}_{\vec{p}}^T \underline{V}_{\vec{y}}^{-1} \underline{G}_{\vec{p}})^{-1}$$

Non-linear model (1st order Taylor)

$$f(\vec{x}, \vec{p}) \cong f(\vec{x}, \vec{p}') + \underline{G}_{p'} (\vec{p} - \vec{p}')$$

$\vec{p}'$: first estimate

$$(\vec{p} - \vec{p}') = \underline{V}_{\vec{p}'} \underline{G}_{\vec{p}'}^T \underline{V}_{\vec{y}}^{-1} (\vec{z} - f(\vec{x}, \vec{p}'))$$

$$\underline{V}_{\vec{p}} = (\underline{G}_{\vec{p}'}^T \underline{V}_{\vec{y}}^{-1} \underline{G}_{\vec{p}'})^{-1}$$

$$\left.\begin{array}{l} \vec{p}' = \vec{p} \\ \underline{V}_{\vec{p}'} = \underline{V}_{\vec{p}} \end{array}\right\}$$

solved by iteration, requires first estimate

LSQ : non-linear model (example)

Input from experiment : $(\vec{x}, \vec{y})$ $\quad V_{\vec{y}}$

Model : $\vec{Y} = f(\vec{X}, \vec{p})$

Minimize : $\chi^2(\vec{p}) = (\vec{y} - f(\vec{x},\vec{p}))^T \underline{V}_{\vec{y}}^{-1} (\vec{y} - f(\vec{x},\vec{p}))$

Non-linear model (1st order Taylor)

$$f(\vec{x},\vec{p}) \cong f(\vec{x},\vec{p}') + \underline{G}_{p'}(\vec{p} - \vec{p}') \qquad g_{p,ij} = \frac{\partial f_i}{\partial p_j}$$

$\vec{p}'$: first estimate

$$(\vec{p} - \vec{p}') = \underline{V}_{\vec{p}'} \underline{G}^T_{\vec{p}'} \underline{V}^{-1}_{\vec{y}} (\vec{z} - f(\vec{x},\vec{p}'))$$

$$\underline{V}_{\vec{p}} = (\underline{G}^T_{\vec{p}'} \underline{V}^{-1}_{\vec{y}} \underline{G}_{\vec{p}'})^{-1}$$

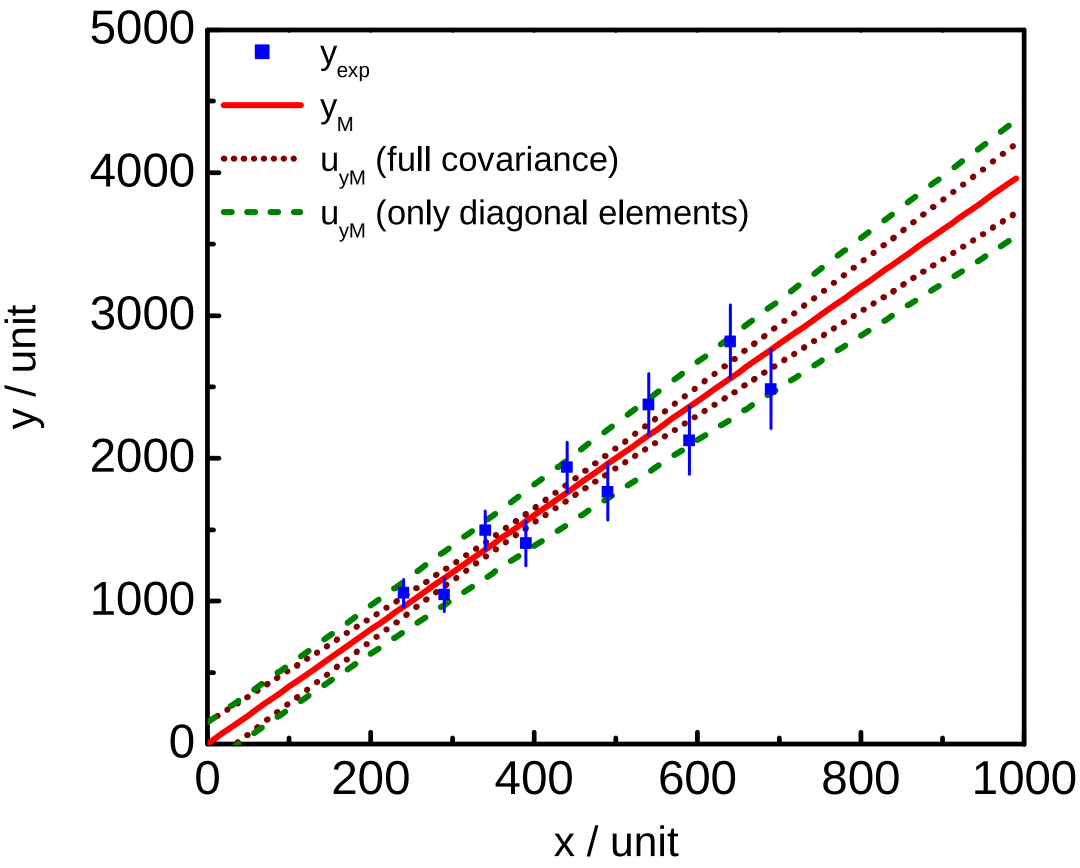
$$\left. \begin{aligned} \vec{p}' &= \vec{p} \\ \underline{V}_{\vec{p}'} &= \underline{V}_{\vec{p}} \end{aligned} \right\}$$

solved by iteration, requires first estimate

$$\vec{Y} = a_0 + a_1 \vec{X}^{a_2} \qquad \vec{p} = (a_o, a_1, a_2)$$

$$\underline{G}_{\vec{p}} = \begin{bmatrix} 1 & x_1^{a_2} & a_1 x_1^{a_2} \ln x_1 \\ 1 & x_2^{a_2} & a_1 x_2^{a_2} \ln x_2 \\ . & . & . \\ . & . & . \\ . & . & . \\ 1 & x_n^{a_2} & a_1 x_n^{a_2} \ln x_n \end{bmatrix}$$

Example: $Y = a_0 + a_1 X$



$$\vec{Y} = \underline{G}_{\vec{p}}\,\vec{p}$$

$$\chi^2(\vec{p}) = (\vec{y} - f(\vec{x},\vec{p}))^T\,\underline{V}_{\vec{y}}^{-1}\,(\vec{y} - f(\vec{x},\vec{p}))$$

$$\vec{p} = V_{\vec{p}}\,\underline{G}_{\vec{p}}^T\,\underline{V}_{\vec{y}}^{-1}\,\vec{y} \qquad g_{p,ij} = \frac{\partial f_i}{\partial p_j}$$

$$\underline{V}_p = (\underline{G}_{\vec{p}}^T\,\underline{V}_{\vec{y}}^{-1}\,\underline{G}_{\vec{p}})^{-1}$$

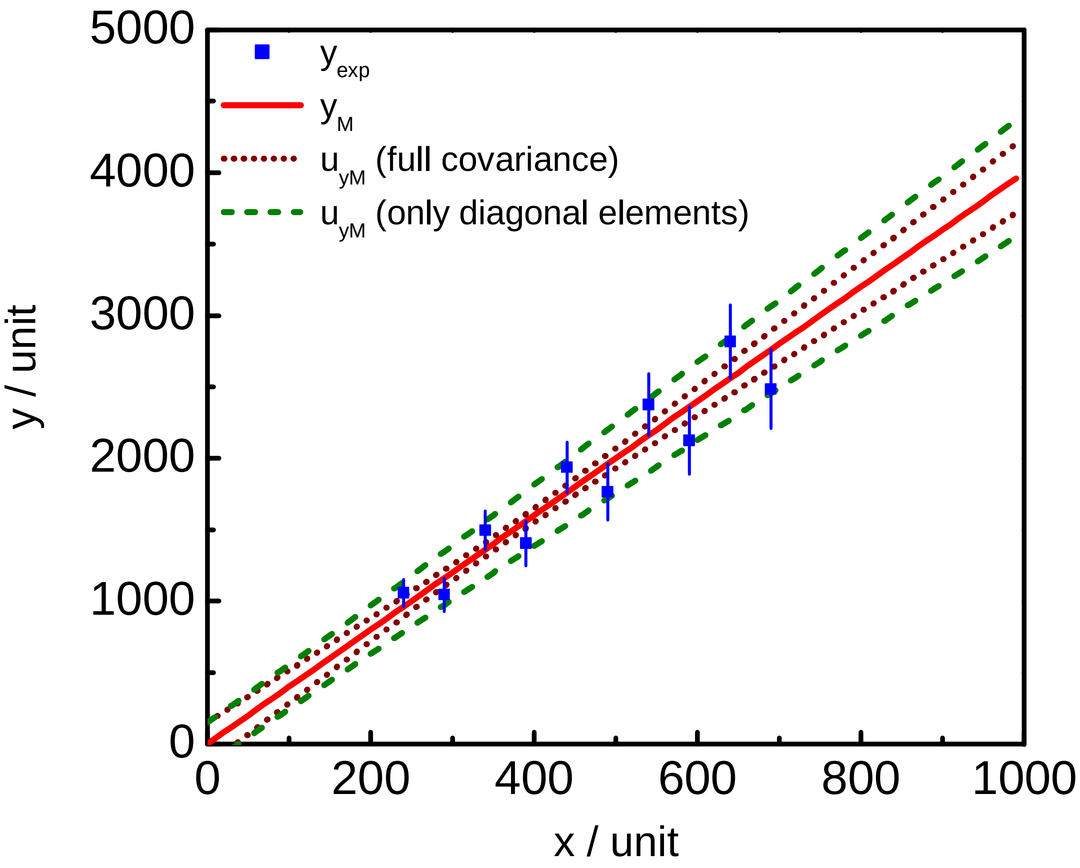
$$\underline{V}_{\vec{y}_M} = \underline{G}_{\vec{p}}\,V_{\vec{p}}\,\underline{G}_{\vec{p}}^T$$

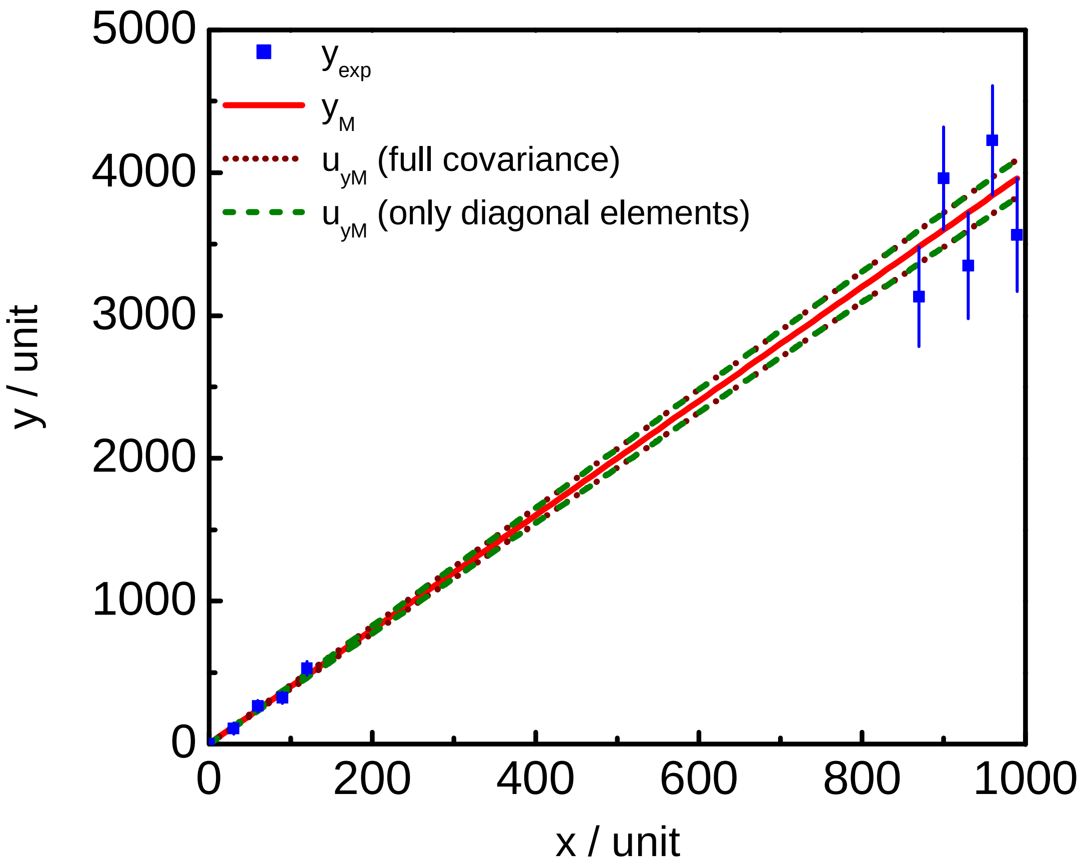
V_p : Only diagonal terms

$$a_0 = 1 \pm 150$$
$$a_1 = 4.00 \pm 0.38$$
$$\rho(a_o, a_1) = 0$$

$$\underline{V}_{(a_0,a_1)} = \begin{bmatrix} 22608 & 0 \\ 0 & 0.146 \end{bmatrix}$$

Example: $Y = a_0 + a_1 X$

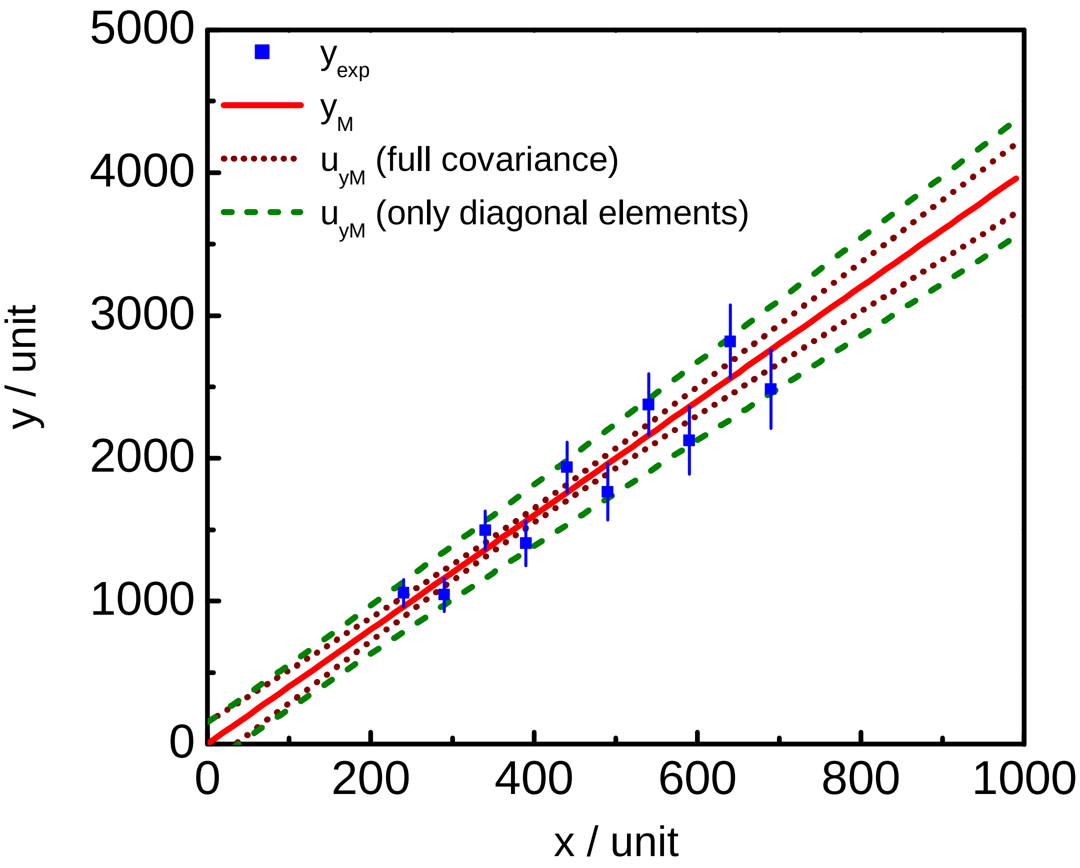




$$a_0 = 1 \pm 150$$
$$a_1 = 4.00 \pm 0.38$$
$$\rho(a_o, a_1) = -0.94$$

$$a_0 = 1.00 \pm 0.10$$
$$a_1 = 4.00 \pm 0.13$$
$$\rho(a_o, a_1) = -0.006$$

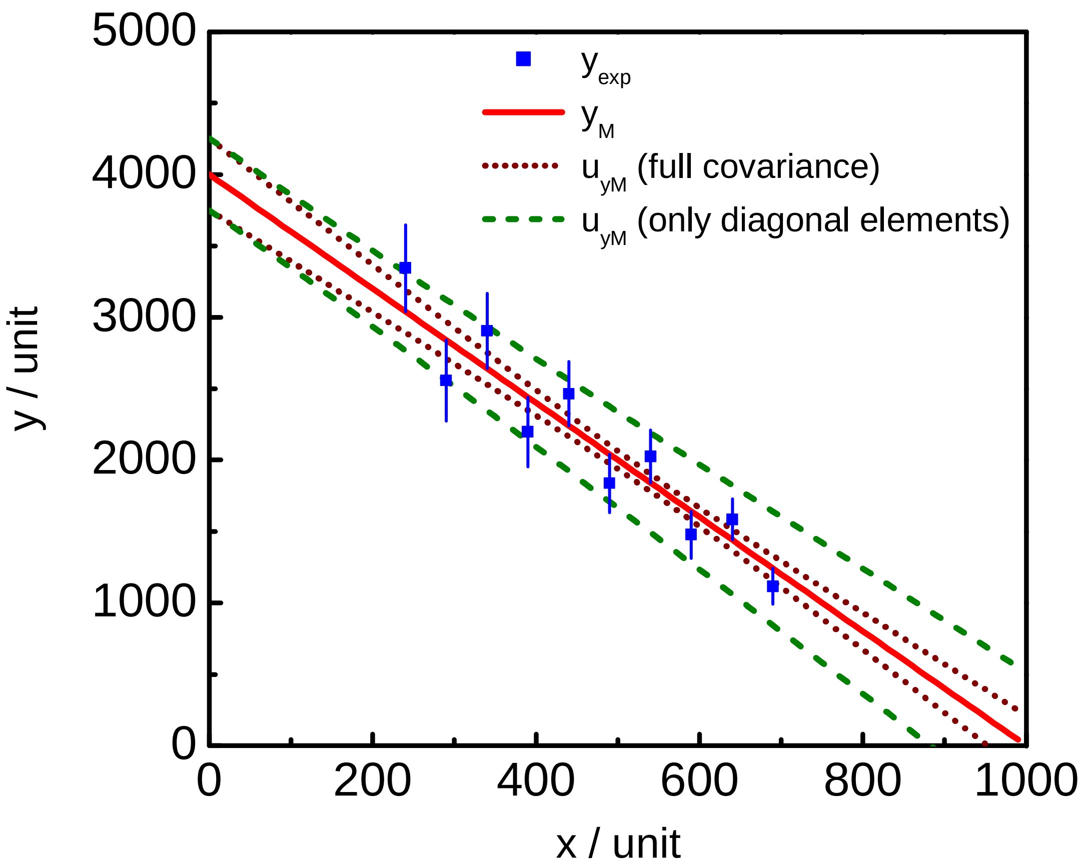
Example: $Y = a_0 + a_1 X$



$$a_0 = 1 \pm 150$$

$$a_1 = 4.00 \pm 0.38$$

$$\rho(a_o, a_1) = -0.94$$



$$a_0 = 4001 \pm 251$$

$$a_1 = 4.00 \pm 0.45$$

$$\rho(a_o, a_1) = -0.971$$

Generalized Least Squares Adjustment (GLSQ)

$$\vec{Y} = \underline{G}_{\vec{p}}\, \vec{p}$$

$$\chi^2(\vec{p})_{min} = (\vec{y} - f(\vec{x},\vec{p}))^T\, \underline{V}_{\vec{y}}^{-1}\, (\vec{y} - f(\vec{x},\vec{p}))$$

$$\vec{p} = V_{\vec{p}}\, \underline{G}_{\vec{p}}^T\, \underline{V}_{\vec{y}}^{-1}\, \vec{y}$$

$$\underline{V}_p = (\underline{G}_{\vec{p}}^T\, \underline{V}_{\vec{y}}^{-1}\, \underline{G}_{\vec{p}})^{-1}$$

Generalized Least Squares (GLSQ)
Account for

- Uncertainties on $\vec{x}$
- Include prior information on model parameters $\vec{p}$

F.H. Fröhner, "Evaluation and Analysis of Nuclear Resonance Data", https://www.oecd-nea.org/dbdata/nds_jefreports/jefreport-18/jeff18.pdf

F.H. Fröhner, "Assigning uncertainties to scientific data", Nucl. Sci. Eng. 126 (1997) 1 -18

GLSQ : + uncertainties on $\vec{x}$

$$\vec{z}_M = h(\vec{q}) = h(\vec{x},\vec{p})$$

$$\chi^2(\vec{q})_{min} = (\vec{z} - h(\vec{x},\vec{p}))^T \underline{V}_{\vec{z}}^{-1} (\vec{z} - h(\vec{x},\vec{p}))$$

$$(\vec{q} - \vec{q}') = \underline{V}_{\vec{q}'} \underline{G}_{\vec{q}'}^T \underline{V}_{\vec{z}}^{-1} (\vec{z} - h(\vec{q}'))$$

$$\underline{V}_{\vec{q}} = (\underline{G}_{\vec{q}'}^T \underline{V}_{\vec{z}}^{-1} \underline{G}_{\vec{q}'})^{-1}$$

$$\left.\begin{aligned} \vec{q}' &= \vec{q} \\ \underline{V}_{\vec{q}'} &= \underline{V}_{\vec{q}} \end{aligned}\right\}$$

solved by iteration

Account for $(\vec{x}, V_{\vec{x}})$ and $(\vec{y}, V_{\vec{y}})$

- Include $(\vec{x}, V_{\vec{x}})$ as experimental input

$$\vec{z} = (\vec{x}, \vec{y}) \qquad V_{\vec{z}} \text{ defined by } (V_{\vec{x}}, V_{\vec{y}})$$

- Include $\vec{x}$ as a model parameter

$$\vec{q} = (\vec{x}, \vec{p})$$

$$h(\vec{q}) = \begin{cases} \vec{x} = \vec{x} \\ \vec{y} = f(\vec{y}, \vec{p}) \end{cases}$$

GLSQ : + uncertainties on $\vec{x}$

Example: $(x_1,y_1), (x_2,y_2), (x_3,y_3) + (V_{\vec{x}}, V_{\vec{y}})$ $\quad \vec{Y}_M = a_0 + a_1 \vec{X}$

- Include $(\vec{x}, V_x)$ as experimental input data

$$\vec{z} = (\vec{x}, \vec{y}) \qquad \underline{V}_{\vec{z}} = \begin{bmatrix} u_{x_1}^2 & 0 & 0 & 0 & 0 & 0 \\ 0 & u_{x_2}^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & u_{x_3}^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & u_{y_1}^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & u_{y_2}^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & u_{y_3}^2 \end{bmatrix}$$

- Include $\vec{x}$ as a model parameter : $\vec{q} = (\vec{x}, \vec{p})$

$$h(\vec{q}) = \begin{cases} \vec{x} = \vec{x} \\ \vec{y} = f(\vec{x}, \vec{p}) \end{cases} \qquad \underline{G}_{\vec{q}} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ a_1 & 0 & 0 & 1 & x_1 \\ 0 & a_1 & 0 & 1 & x_2 \\ 0 & 0 & a_1 & 1 & x_3 \end{bmatrix}$$

$$(\vec{q} - \vec{q}\,') = \underline{V}_{\vec{q}\,'} \, \underline{G}_{\vec{q}\,'}^T \, \underline{V}_{\vec{z}}^{-1} \, (\vec{z} - h(\vec{q}\,'))$$

$$\underline{V}_{\vec{q}} = (\underline{G}_{\vec{q}\,'}^T \, \underline{V}_{\vec{z}}^{-1} \, \underline{G}_{\vec{q}\,'})^{-1}$$

$$\left.\begin{aligned} \vec{q}\,' &= \vec{q} \\ \underline{V}_{\vec{q}\,'} &= \underline{V}_{\vec{q}} \end{aligned}\right\} \text{solved by iteration}$$

GLSQ : + uncertainties on $\vec{x}$ + prior ($\vec{p}_0$, $V_{\vec{p}0}$)

Example: $(x_1,y_1),\ (x_2,y_2),\ (x_3,y_3)\ +\ (V_{\vec{x}},V_{\vec{y}})$ $\qquad \vec{Y}_M = a_0 + a_1\vec{X} \qquad (a_0,a_1)\ +\ V_{\vec{a}}$

- Include ($\vec{x}$,V_x) and prior ($\vec{p}_0$,V_{p0}) as input data

$$\vec{z} = (\vec{p},\vec{x},\vec{y}) \qquad \underline{V}_{\vec{z}} = \begin{bmatrix} u^2_{a_0} & v_{a_0,a_1} & 0 & 0 & 0 & 0 & 0 & 0 \\ v_{a_0,a_1} & u^2_{a_1} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & u^2_{x_1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & u^2_{x_2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & u^2_{x_3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & u^2_{y_1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & u^2_{y_2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & u^2_{y_3} \end{bmatrix}$$

- Include $\vec{x}$ as a model parameter : $\vec{q} = (\vec{x}, \vec{p})$

$$h(\vec{q}) = \begin{cases} \vec{x} = \vec{x} \\ \vec{y} = f(\vec{x},\vec{p}) \end{cases} \qquad \underline{G}_{\vec{q}} = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ a_1 & 0 & 0 & 1 & x_1 \\ 0 & a_1 & 0 & 1 & x_2 \\ 0 & 0 & a_1 & 1 & x_3 \end{bmatrix}$$

$$(\vec{q}-\vec{q}') = \underline{V}_{\vec{q}'}\,\underline{G}^T_{\vec{q}'}\,\underline{V}^{-1}_{\vec{z}}\,(\vec{z}-h(\vec{q}'))$$

$$\underline{V}_{\vec{q}} = (\underline{G}^T_{\vec{q}'}\,\underline{V}^{-1}_{\vec{z}}\,\underline{G}_{\vec{q}'})^{-1}$$

$$\left.\begin{aligned} \vec{q}' &= \vec{q} \\ \underline{V}_{\vec{q}'} &= \underline{V}_{\vec{q}} \end{aligned}\right\}$$ solved by iteration

GLSQ

Input from experiment : $(\vec{x},\vec{y})\quad (\underline{V}_{\vec{x}},\underline{V}_{\vec{y}})\ +\ (\vec{p}_0,\underline{V}_{\vec{p}_0})$

Model : $\vec{Z} = h(\vec{q}) = h(\vec{X},\vec{p})$

Minimize : $\chi^2(\vec{q}) = (\vec{z}-h(\vec{q}))^T\,\underline{V}_{\vec{z}}^{-1}\,(\vec{z}-h(\vec{q}))$

$\vec{z} = (\vec{p}_0,\vec{x},\vec{y})\qquad V_{\vec{z}}$ defined by $(V_{\vec{p}_0}, V_{\vec{x}}, V_{\vec{y}})$

$$h(\vec{q}) = \begin{cases}\vec{p} = \vec{p}\\ \vec{X} = \vec{X}\\ \vec{Y} = f(\vec{X},\vec{p})\end{cases}$$

Generalized least squares fit (GLSQ)

$$h(\vec{q}) \cong h(\vec{q}\,') + \underline{G}_{\vec{q}\,'}(\vec{q}-\vec{q}\,')\qquad g_{p,ij} = \frac{\partial h_i}{\partial q_j}$$

$\vec{q}\,'$: first estimate

Accounts for:

- Uncertainty on all experimental quantities
- Prior information on model parameters
- Correlation between all exp. quantities

$x \Leftrightarrow y$

$p_0 \Leftrightarrow x$

$p_0 \Leftrightarrow y$

$$(\vec{q}-\vec{q}\,') = \underline{V}_{\vec{q}\,'}\,\underline{G}_{\vec{q}\,'}^T\,\underline{V}_{\vec{z}}^{-1}\,(\vec{z}-h(\vec{q}\,'))$$

$$\underline{V}_{\vec{q}} = (\underline{G}_{\vec{q}\,'}^T\,\underline{V}_{\vec{z}}^{-1}\,\underline{G}_{\vec{q}\,'})^{-1}$$

$$\left.\begin{aligned}\vec{q}\,' &= \vec{q}\\ \underline{V}_{\vec{q}\,'} &= \underline{V}_{\vec{q}}\end{aligned}\right\}$$

solved by iteration, requires first estimate

Bayesian theory

Input from experiment : $(\vec{x}, \vec{y}) \quad V_{\vec{y}} \quad + (\vec{p}_0, \underline{V}_{\vec{p}_0})$

Model : $\vec{Y} = f(\vec{X}, \vec{p})$

Bayes' theorem : $P(H|D\,J) \propto P(D|H\,J)\,P(H|J)$

$(\vec{y}, \underline{V}_{\vec{y}})$ → $P(D|H\,J)$; $(\vec{p}_0, \underline{V}_{\vec{p}_0})$ → $P(H|J)$

H : model parameters
D : experimental data
J : model

no correlation between prior and updating experimental data

$$f(\vec{x},\vec{p}) \cong f(\vec{x},\vec{p}\,') + \underline{G}_{\vec{p}\,'}(\vec{p} - \vec{p}\,') \qquad g_{p',ij} = \frac{\partial f_i}{\partial p'_j}$$

$$\vec{p} = \vec{p}_o + V_{\vec{o}}\, \underline{G}^T_{\vec{p}\,'} (\underline{G}_{\vec{p}\,'}\, V_{\vec{o}}\, \underline{G}^T_{\vec{p}\,'} + \underline{V}_{\vec{y}})^{-1} (z - (f(\vec{x},\vec{p}\,') + \underline{G}_{\vec{p}\,'}(\vec{p}_o - \vec{p}\,')))$$

$$\underline{V}_{\vec{p}} = V_{\vec{o}} - V_{\vec{o}}\, \underline{G}^T_{\vec{p}\,'} (\underline{G}_{\vec{p}\,'}\, V_{\vec{o}}\, \underline{G}^T_{\vec{p}\,'} + \underline{V}_{\vec{y}})^{-1} \underline{G}_{\vec{p}\,'}\, V_{\vec{o}}$$

$$\left.\begin{array}{l} \vec{p}\,' = \vec{p} \\ \underline{V}_{\vec{p}\,'} = \underline{V}_{\vec{p}} \end{array}\right\}$$

solved by iteration

Propagation of uncertainties by CUP

Conventional uncertainty propagation (CUP)

GLUP

$$\underline{V}_Z = \underline{G}_X \, \underline{V}_X \, \underline{G}_X^T$$

GLSQ

$$(\vec{q} - \vec{q}\,') = \underline{V}_{\vec{q}\,'} \, \underline{G}_{\vec{q}\,'}^T \underline{V}_{\vec{z}}^{-1} \, (\vec{z} - h(\vec{q}\,'))$$

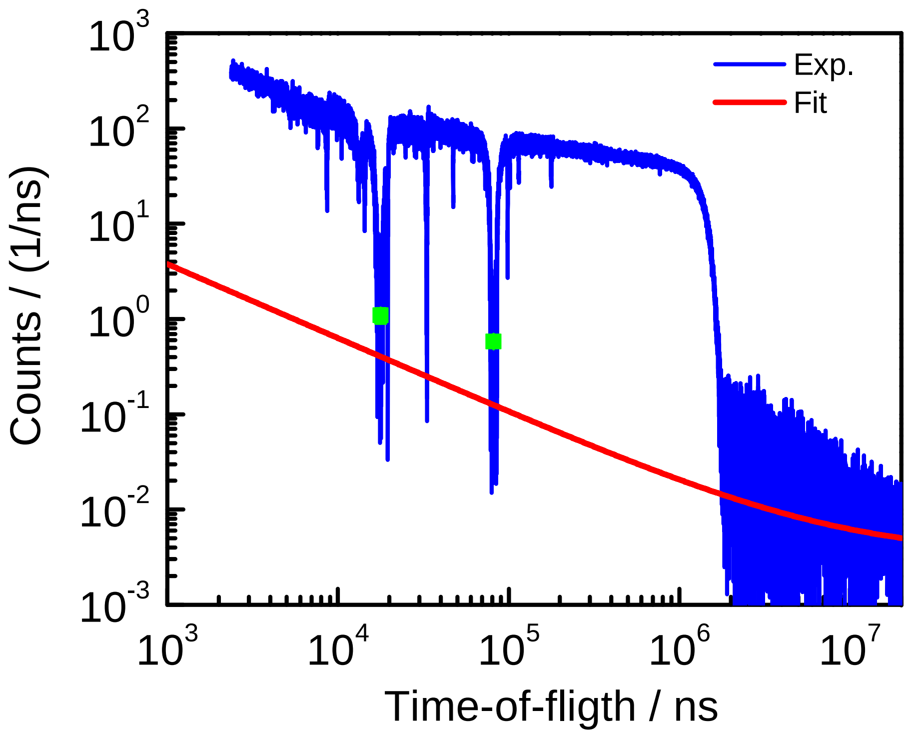
$$\underline{V}_{\vec{q}} = (\underline{G}_{\vec{q}\,'}^T \underline{V}_{\vec{z}}^{-1} \, \underline{G}_{\vec{q}\,'})^{-1}$$

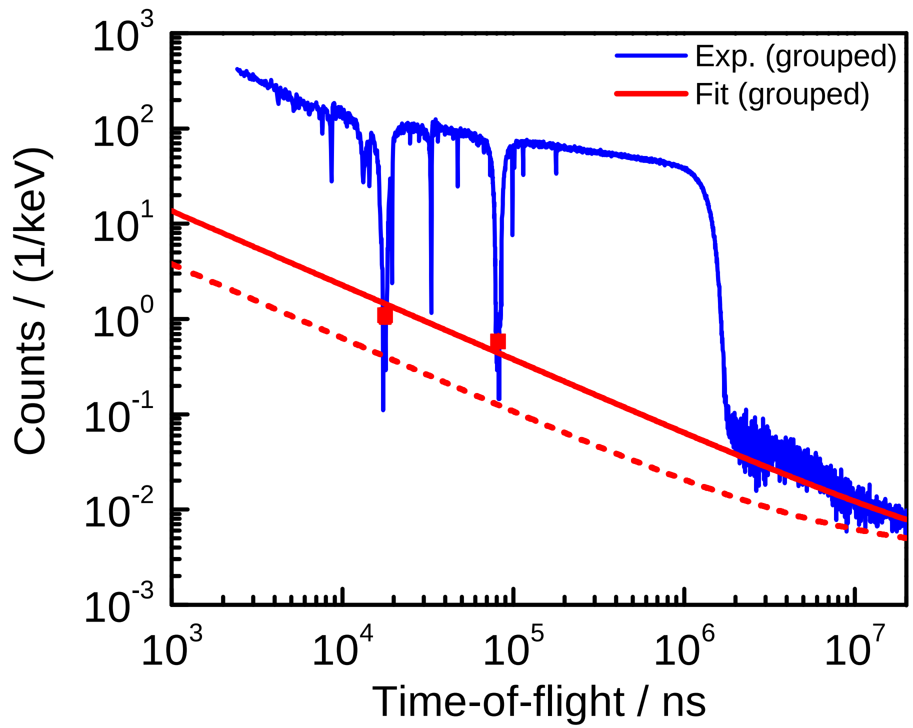
Based on

- **Normal (Gaussian) PDF's**
- **Linear problem (1st order Taylor development)**

Example : background fit

$$B(t) = b_o + b_1 t^{b_2}$$





⇒ limited number of counts per time channel
⇒ Uncertainties not well defined by $u_C = \sqrt{C}$
⇒ Poison cannot be approximated by normal

⇒ grouped data
⇒ Poison can be approximated by normal

Example

(y_1,u_{y_1}) , (y_2,u_{y_2}) : independent experimental observables of Y

(k,u_k) : experimental observable of K, independent of (y_1,y_2)

$$y_1 = 1.00 \pm 0.10$$

$$y_2 = 1.50 \pm 0.15$$

$$k = 1.00 \pm 0.20$$

Determine best estimate of Z = KY

$$(y_1,y_2,k) \Rightarrow \langle z \rangle = \langle ky \rangle$$

Solutions

A) $(y_1, y_2, k) \underset{\text{GLSQ}}{\Rightarrow} (\bar{y}, k) \Rightarrow z = k\,\bar{y}$

B) $(y_1, y_2, k) \Rightarrow (z_1, z_2) \underset{\text{GLSQ}}{\Rightarrow} \bar{z}$

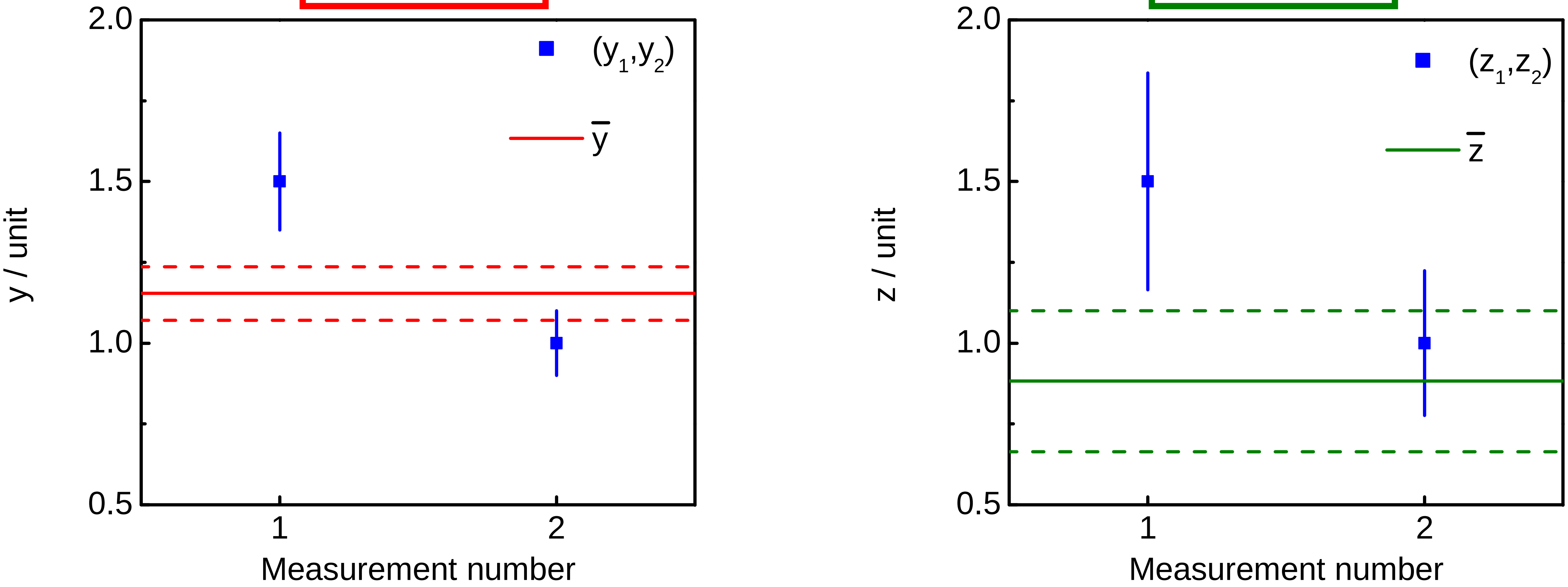
Solutions

A) $(y_1, y_2, k) \underset{\text{GLSQ}}{\Rightarrow} (\bar{y}, k) \Rightarrow z = k\,\bar{y}$

B) $(y_1, y_2, k) \Rightarrow (z_1, z_2) \underset{\text{GLSQ}}{\Rightarrow} \bar{z}$

1.154 ± 0.245

0.882 ± 0.218



Peelle's Pertinent Puzzle

Problem:

G. D'Agostini, NIM. A346 (1994) 306
D. Neudecker et al., NSE, 170 (2012), 54 - 60

$$\bar{z} = k\,\bar{y} \qquad \bar{z} = \frac{z_1\sigma_{y_2}^2 + z_2\sigma_{y_1}^2}{\sigma_{y_1}^2 + \sigma_{y_2}^2 + \boxed{\frac{\sigma_k^2}{k^2}(y_1 - y_2)^2}}$$

not well defined covariance matrix

Solution: include the correction factor K as a model parameter and additional experimental input data

Zhao & Perey ORNL/TM-12106
D'Agostini, NIM A346 (1994) 306
Fröhner, NSE 126 (1997) 1 - 18

$$(\vec{y},k) = f(z,k) = \begin{cases} y_1 = \dfrac{z}{k} \\ y_2 = \dfrac{z}{k} \\ k = k \end{cases}$$

Solution for PPP

- Experimental input

$$(\vec{y},k) = (1.00, 1.00, 1.50) \qquad \underline{V}_{y_1,y_2,k} = \begin{bmatrix} 0.10^2 & 0 & 0 \\ 0 & 0.15^2 & 0 \\ 0 & 0 & 0.20^2 \end{bmatrix}$$

- Model

$$\chi^2(z_0,k_0) = ((y_1,y_2,k) - f(z_0,k_0))^T \, \underline{V}^{-1}_{y_1,y_2,k} \, ((y_1,y_2,k) - f(z_0,k_0))$$

$$(\vec{y},k) = f(z,k) = \begin{cases} y_1 = \dfrac{z}{k} \\ y_2 = \dfrac{z}{k} \\ k = k \end{cases}$$

$$z_0 = 1.154 \pm 0.245 \qquad k_0 = 1.00 \pm 0.20 \qquad \underline{\rho} = \begin{bmatrix} 1 & 0.94 \\ 0.94 & 1 \end{bmatrix}$$

Least squares on (y_1,y_2) and applying correction factor afterwards : $z_o = 1.154 \pm 0.245$

Definitions and terminology

International vocabulary of metrology

Basic and general concepts and associated terms (VIM)

(JCGM 200:2012)

Evaluation of Measurement data

Guide to the expression of uncertainty in measurement

(JCGM 100 :2008)

http://www.bipm.org/en/bipm/

Definitions and terminology

- Error ⇔ Uncertainty

- Precision ⇔ Accuracy

- Reporting of uncertainty
  - Standard ⇔ expanded
  - Combined uncertainty
  - Correlated ⇔ uncorrelated

Measurement error and uncertainty

- **Measurement error :** difference between two values

  "result of a measurement minus a true value of the measurand "

  can be + or -

error ≠ uncertainty

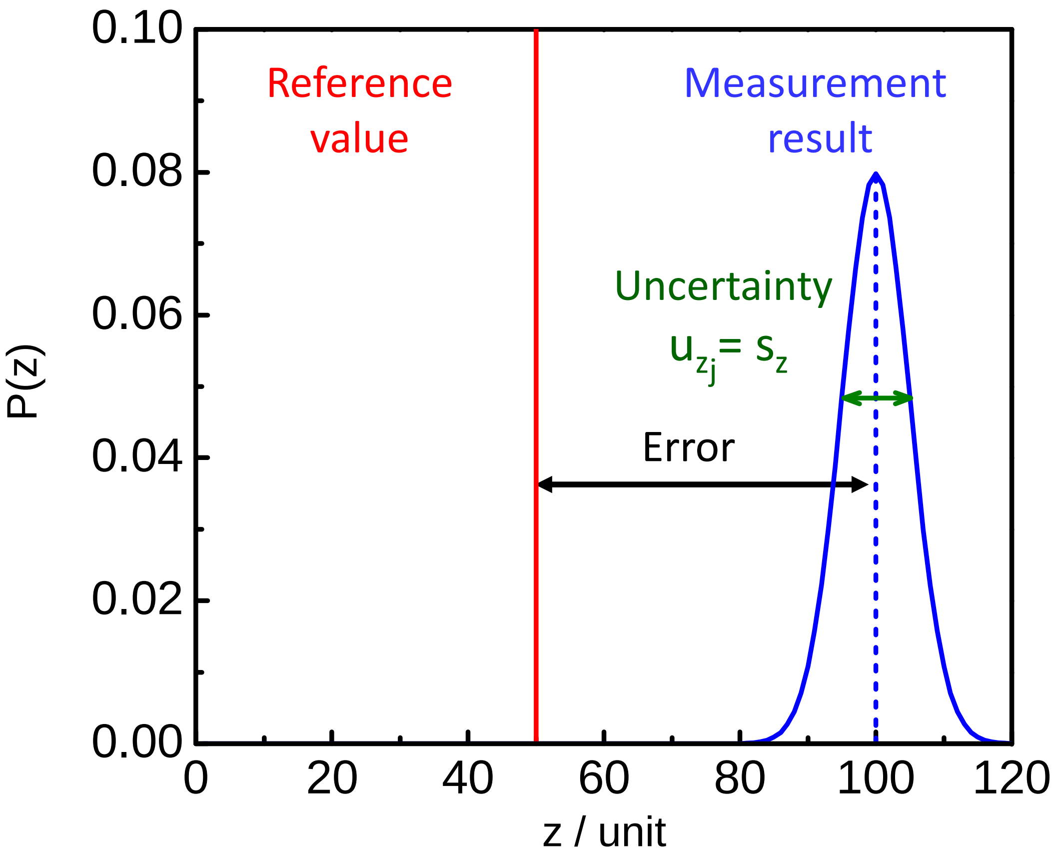
- **Measurement uncertainty :** dispersion of a distribution

  *"**non-negative parameter** characterizing the dispersion of the values being attributed to the measurand"*

  always > 0

  determined by the width of the PDF of the error component(s)

Measurement error and uncertainty



- **Measurement error**

  Difference between values

  + or -

- **Uncertainty**

  Derived from width of a distribution

  > 0

GLUP : (Y,B) ⇒ estimate of Z = Y - B

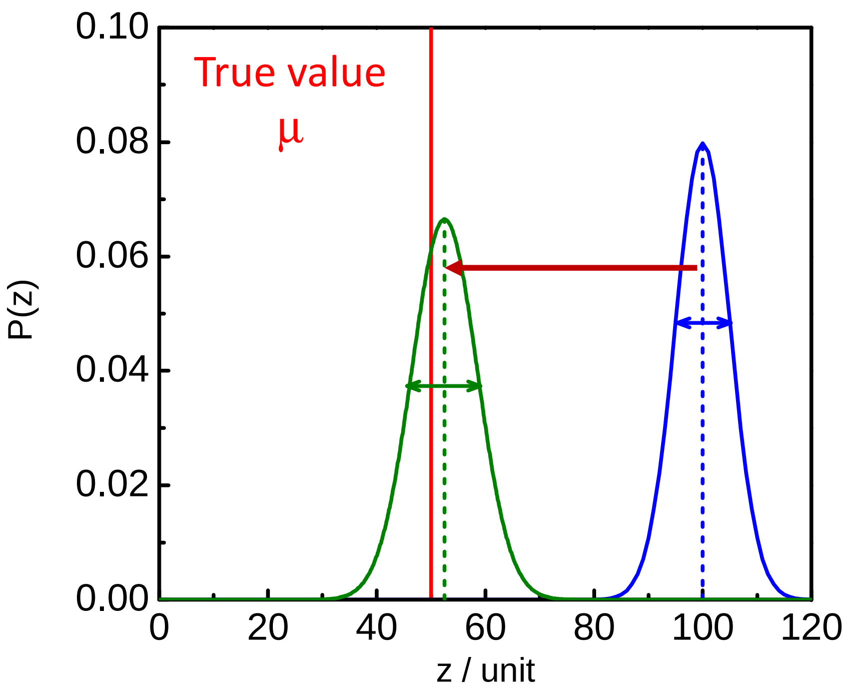
Z : measurand, i.e. quantity of interest, with true value μ

Y : result of an experiment to estimate true value of Z

all measurements in same conditions (e.g. measurement time,…)

B : correction for a known systematic effect (background)

Z = Y-B



$$\bar{y} = \frac{1}{m}\sum_{j=1}^{m} y_j$$

$$u_{y_j}^2 = s_y^2 = \frac{1}{m-1}\sum_{j=1}^{m}(\bar{y} - y_j)^2$$

$$u_{\bar{y}} = \sqrt{\frac{1}{m^2}\sum_j u_{y_j}^2} = \frac{s_y}{\sqrt{m}}$$

$$z = \bar{y} - b \qquad u_{\bar{z}} = \sqrt{\frac{s_y^2}{m} + u_b^2}$$

GLUP : (Y,B) ⇒ estimate of Z = KY

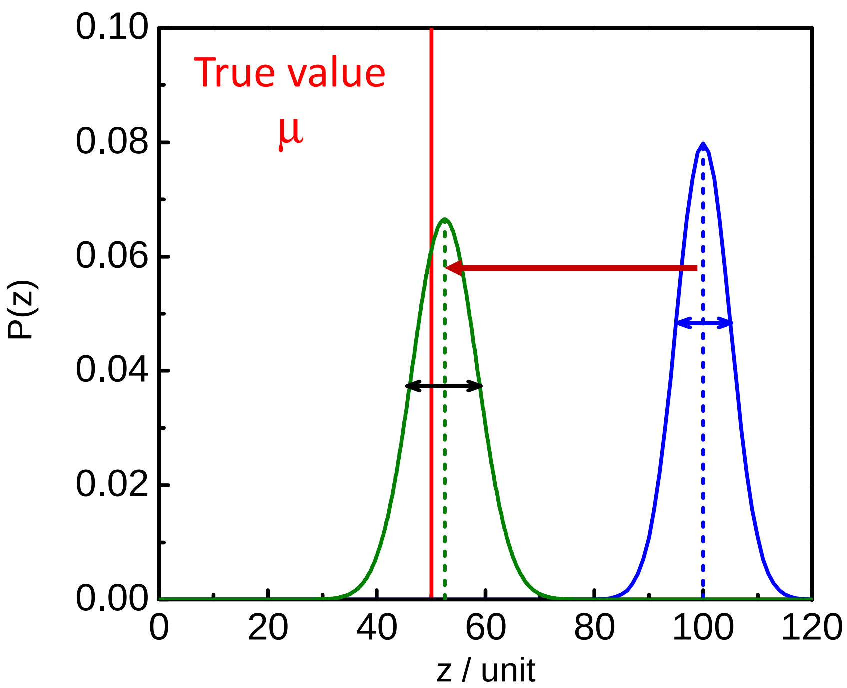
Z : measurand, i.e. quantity of interest, with true value μ

Y : result of an experiment to estimate true value of Z

all measurements in same conditions (e.g. measurement time,…)

K : correction for a known systematic effect (normalization)

Z = K Y



$$\bar{y} = \frac{1}{m}\sum_{j=1}^{m} y_j$$

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$$u_{\bar{y}} = \sqrt{\frac{1}{m^2}\sum_{j} u_{y_j}^2} = \frac{s_y}{\sqrt{m}}$$

$$z = k\,\bar{y} \qquad u_{\bar{z}} = \sqrt{\frac{k^2}{m}s_y^2 + \bar{y}^2 u_k^2}$$

GLUP : (Y,B) ⇒ estimate of Z = KY

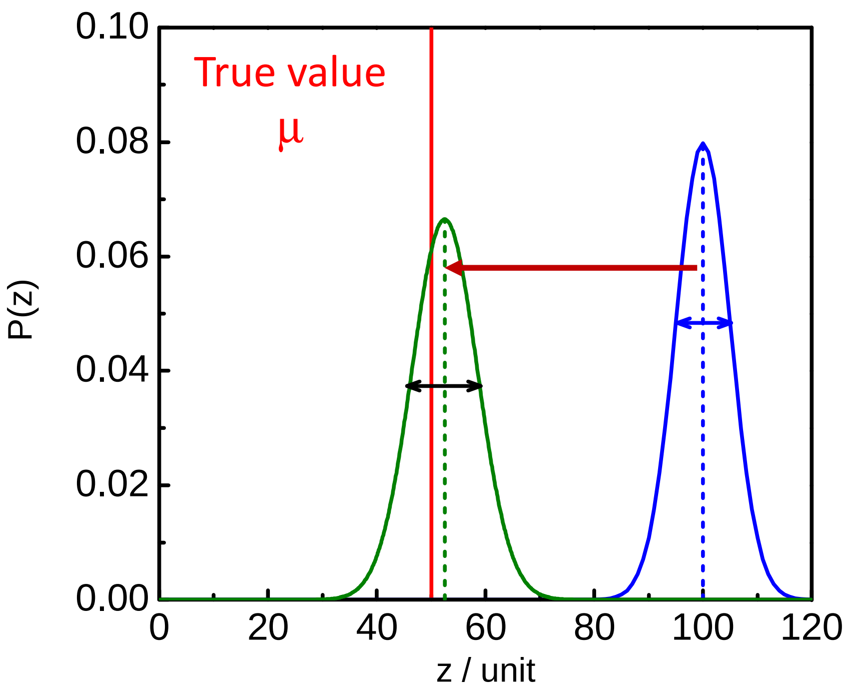
Z : measurand, i.e. quantity of interest, with true value μ

Y : result of an experiment to estimate true value of Z

all measurements in same conditions (e.g. measurement time,…)

K : correction for a known systematic effect (normalization)

Z = K Y



$$\bar{y} = \frac{1}{m}\sum_{j=1}^{m} y_j$$

$$u_{y_j}^2 = s_y^2 = \frac{1}{m-1}\sum_{j=1}^{m}(\bar{y} - y_j)^2$$

$$u_{\bar{y}} = \sqrt{\frac{1}{m^2}\sum_j u_{y_j}^2} = \frac{s_y}{\sqrt{m}}$$

$$z = k\,\bar{y} \qquad \frac{u_{\bar{z}}}{\bar{z}} = \sqrt{\frac{1}{m}\frac{s_y^2}{\bar{y}^2} + \frac{u_k^2}{k^2}}$$

Measurement precision and accuracy

- **Measurement precision**

  "Closeness of the agreement between the results of replicate measurements on the same measurand under specified conditions"

- **Measurement accuracy (related to systematic error)**

  "Closeness of the agreement between the result of a measurement and a true value of the quantity intended to be measured (measurand) "

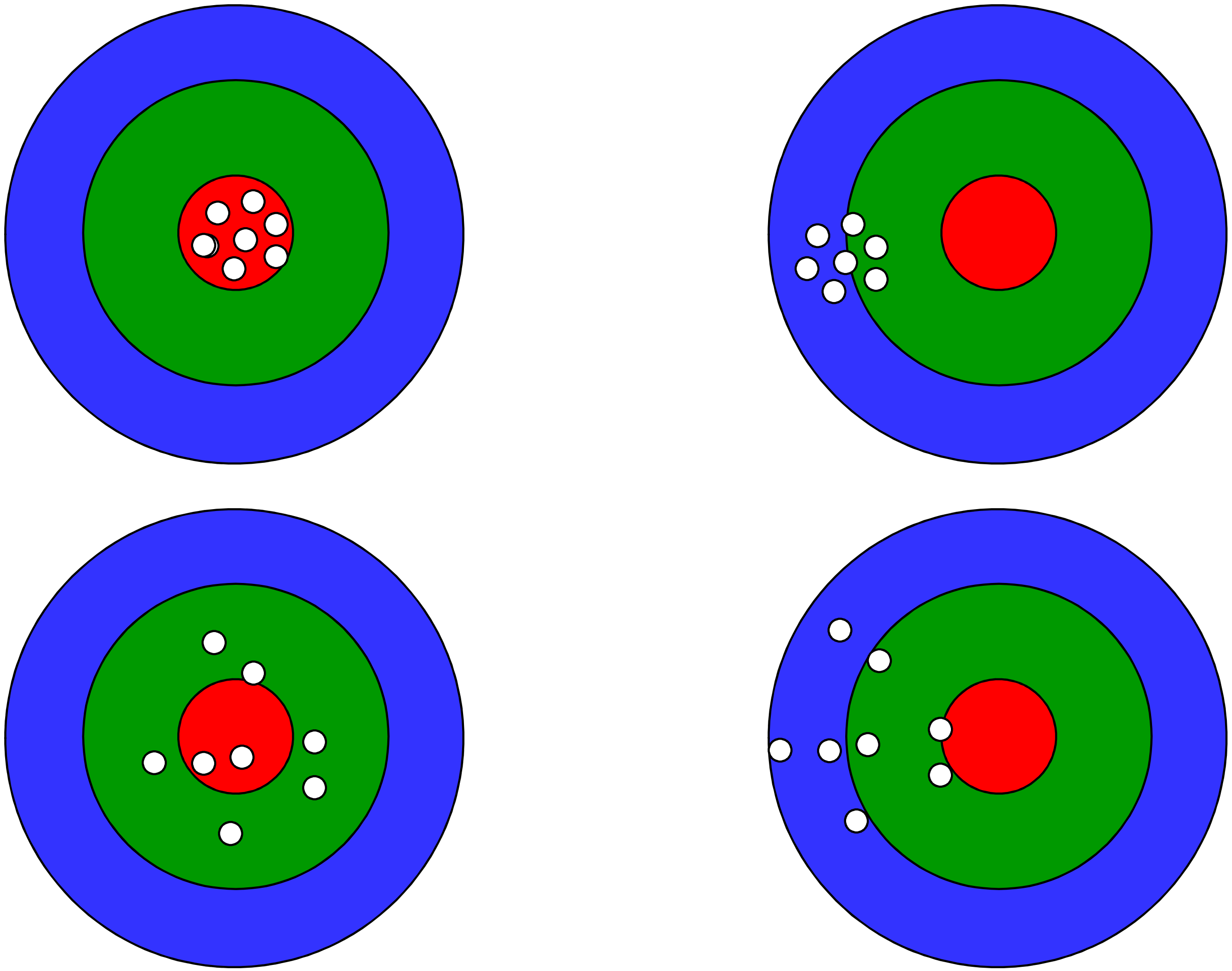
Precision ⇔ Accuracy

Accurate

Inaccurate
(due to a systematic error or bias)

Precise

Imprecise



Standard or expanded uncertainty $x \pm u_x$ with $u_x = \lambda_p \sigma$

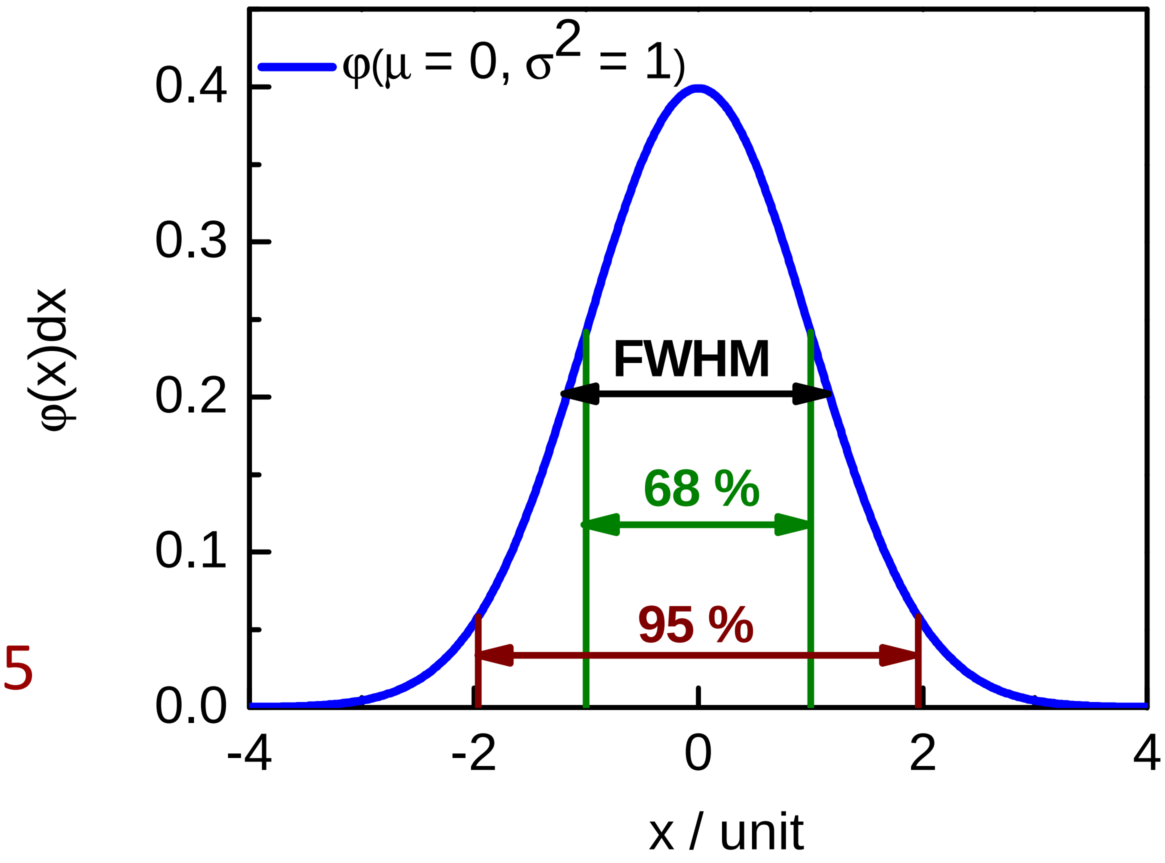
- Standard uncertainty

  $\lambda_p = 1$ with $p = 0.68$

- Expanded uncertainty

  $\lambda_p > 1$

  e.g. $\lambda_p = 1.96 \Rightarrow p = 0.95$



Reporting of uncertainties

(y,u_y), (b,u_b) and (k,u_k) independent input quantities $\Rightarrow$ estimate of Z

$$Z = Y + B \quad \Rightarrow \quad z = y + b \qquad u_z^2 = u_y^2 + u_b^2$$

$$Z = Y - B \quad \Rightarrow \quad z = y - b \qquad u_z^2 = u_y^2 + u_b^2$$

$$Z = K\,Y \quad \Rightarrow \quad z = k\,y \qquad u_z^2 = k^2\,u_y^2 + y^2 u_k^2 \qquad \frac{u_z^2}{z^2} = \frac{u_y^2}{y^2} + \frac{u_k^2}{k^2}$$

$$Z = \frac{Y}{K} \quad \Rightarrow \quad z = \frac{y}{k} \qquad u_z^2 = \frac{u_y^2}{k^2} + \frac{y^2}{k^4} u_k^2 \qquad \frac{u_z^2}{z^2} = \frac{u_y^2}{y^2} + \frac{u_k^2}{k^2}$$

Combined uncertainties

Reliable experimental data and results

Requires

- Understanding of the measurement process (scientific background)
  - experimental observables
  - measurement model
- Well documented experimental observables, including
  - all experimental details (input parameters, systematic effects)
  - all uncertainty components (correlated and uncorrelated)

$\Rightarrow$ Propagation of uncertainties (uncorrelated & correlated) not complicated

GLUP : $\underline{V}_Z = \underline{G}_X \, \underline{V}_X \, \underline{G}_X^T$

GLSQ: $(\vec{q} - \vec{q}') = \underline{V}_{\vec{q}'} \, \underline{G}_{\vec{q}'}^T \underline{V}_{\vec{z}}^{-1} (\vec{z} - h(\vec{q}'))$

$$\underline{V}_{\vec{q}} = (\underline{G}_{\vec{q}'}^T \underline{V}_{\vec{z}}^{-1} \, \underline{G}_{\vec{q}'})^{-1}$$

Note : GLUP & GLSQ based on normal probability distributions

$\Rightarrow$ AGS-formalism (concept)

Topical day organized by SCK•CEN & EC – JRC – IRMM

Generation and use of covariance data in nuclear energy applications

10 – 11 December 2015

Organized by : SCK•CEN and EC – JRC – IRMM

at EC – JRC – IRMM
Retieseweg 111
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http://academy.sckcen.be/en/Events/