Uncertainty calculations and reporting of measurement results

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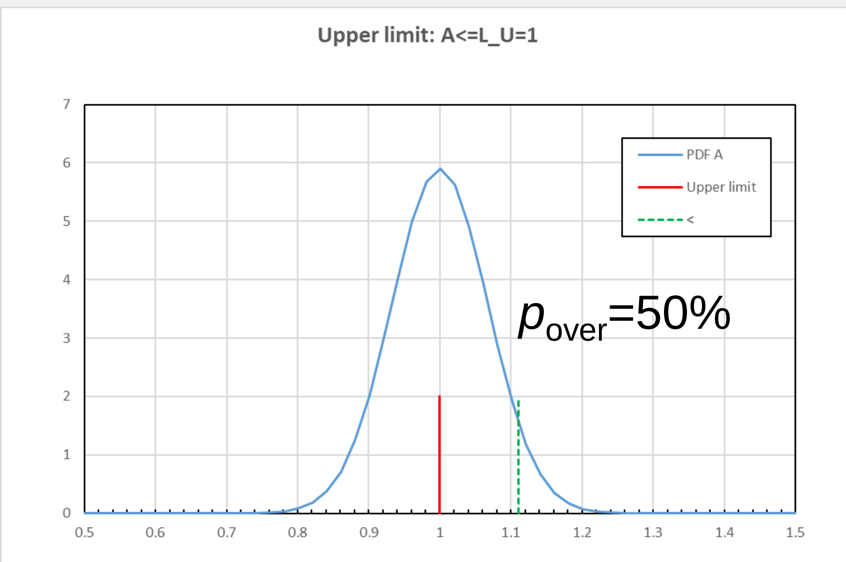
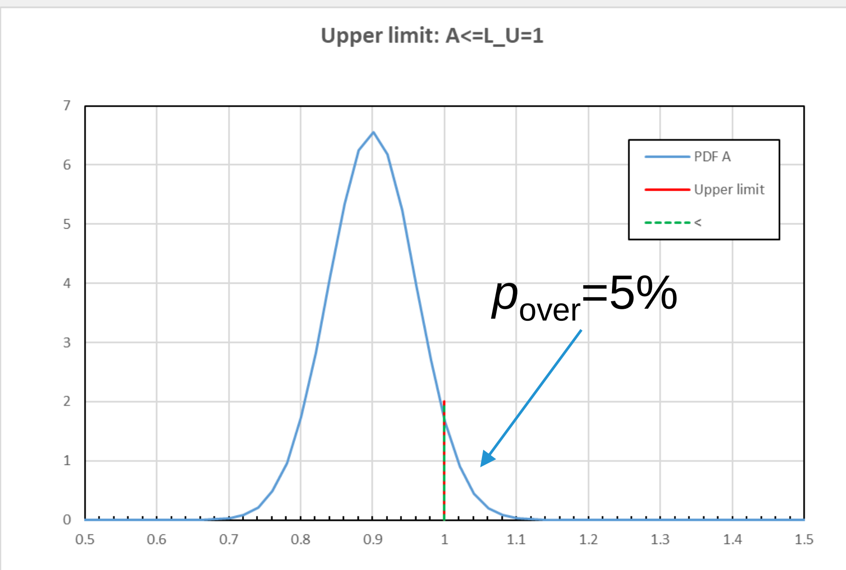
Invited lecture at NKS GammaSkills 2023

Why are measurements done?

- Why are we doing measurements?
- Why is uncertainties important?
- Why should we not overestimate the uncertainty?
- Why should we not underestimate the uncertainty?





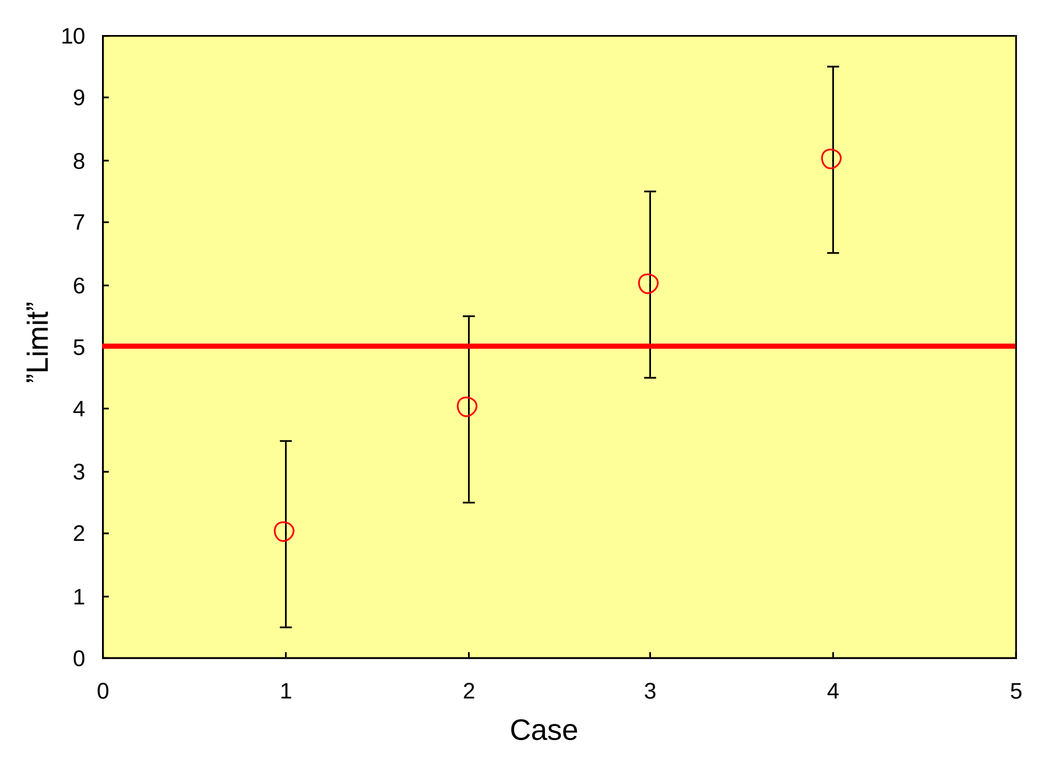
Why measurements?

-Measurement results are used as an essential part in decision making processes!

-Overestimation of the measurement uncertainty may result in higher costs (actions when actions might not be needed)

-Underestimation may result in higher risks… (no actions when actions should have been taken)

(*If the uncertainty is considered in the decision*)



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Decision rules (ISO 17025 7.8.6)

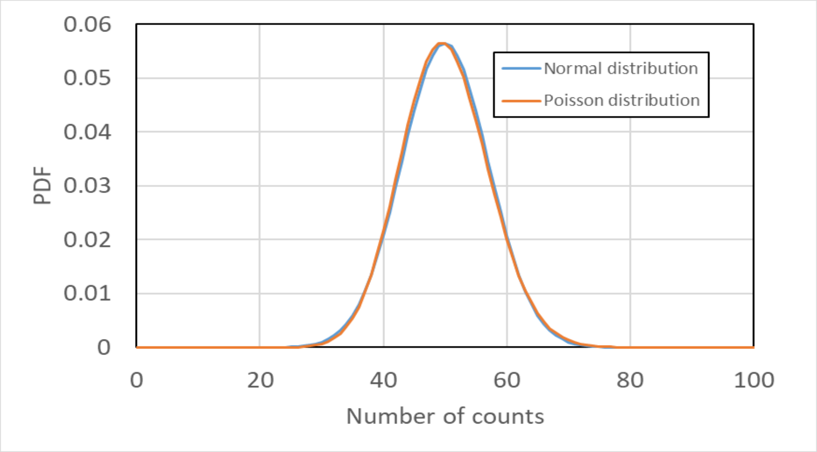
- When a statement about conformity to *e.g.* a regulatory limit is done by a testing laboratory the decision rule used shall be documented taking into account the risk associated with the rule.
- Simple acceptance (mean measurement result compared to limit(s)): 50% risk for a normal probability density function.
  The measurement uncertainty is not considered for this rule
  The most used rule?
- Rule with an accepted maximum risk to be above a limit
- Differences depending on the evaluation method (GUMUF or MC) for non-linear model equations (often the case ”in our world”)
  ➔Inclusion of the evaluation method and assumptions/modelling of input quantities should maybe also be stated?

Basic statistics

- Counting processes are governed by a binomial process (success, no success)
- For normal laboratory measurements the binomial distribution can be approximated with the Poisson distribution (a large number of trials each having a low probability for success)
- If the number of observations is large enough the Poisson distribution can be well approximated by a normal distribution.

Standard deviation of the number of counts *N*:

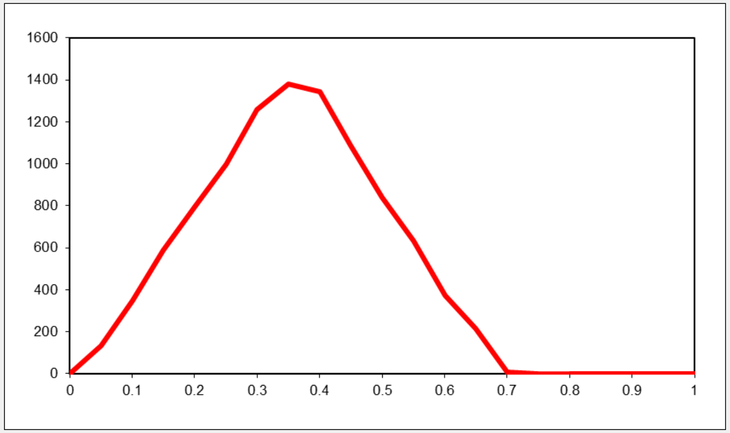
$$\sqrt{N}$$



Basic statistics

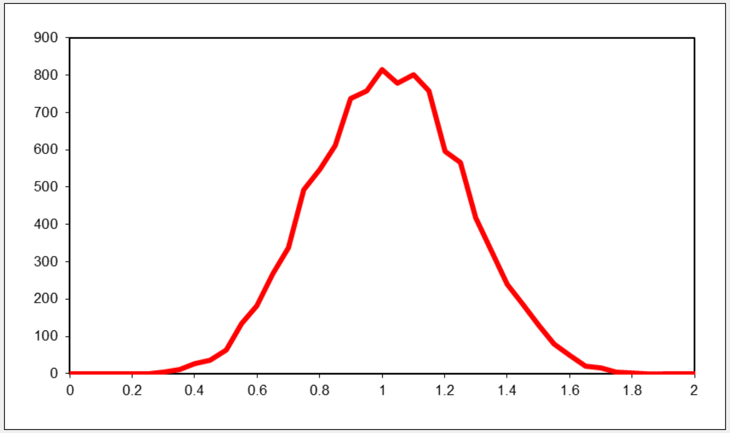
- For a linear combination of distributions (although non-normal), the resulting distribution will eventually be normal:
  -Central Limit Theorem
- After adding *e.g.* a few rectangular distributions you will get an approximate normal distribution:

-Two rectangular distributions having the same width ➔Triangular distribution:



Triangular distribution

-Six rectangular distributions:



Appr. normal distribution

Basic statistics

- Central limit theorem:
  One practical consequence of the Central Limit Theorem is that when the combined standard uncertainty $u_c(y)$ is **not** dominated by one component obtained using a Type A evaluation having a low number of observations *(df* is small*)*, or a Type B evaluation based on *e.g.* a rectangular distribution *y* will be approximately normally distributed

The GUM Uncertainty Framework (uncertainty propagation)

Holds when:

- The model equation is linear (or the uncertainties of non-linear input quantities are ’small enough’)
- The probability distributions of the input quantities are normal

➔The GUMUF gives (almost) exact results
but can otherwise often give results that are fit-for-purpose for most applications…

Basic statistics

Important to know when to use which one of these:

- The *standard deviation* is a measure of the spread between repeated data:

$$s = \sqrt{\frac{(x_1 - \bar{x})^2 + (x_1 - \bar{x})^2 + \ldots + (x_n - \bar{x})^2}{n-1}} = \sqrt{\frac{\sum (x_i - \bar{x})^2}{n-1}}$$

- The *standard deviation of the mean* is a measure of how the average will spread:

$$s(\bar{x}) = \frac{s}{\sqrt{n}}$$

The GUM method

- A generic and straight-forward procedure, which can be applied to all kinds of measurements (radionuclide measurements, chemical measurements,…)
- -ISO Guide 98-3: *Uncertainty in measurements. Guide To The Expression Of Uncertainty In Measurement (GUM:1995)*. International Organization of Standardization, Geneva, Switzerland (*Free version: JCGM 100:2008*)

  -*Quantifying Uncertainty in Analytical Measurement*. EURACHEM/CITAC Guide, 2nd Edition, 2000.
  (*A nice guide applied to chemical measurements*…)

The GUM method: some pros

- You will gain a much deeper understanding, and knowledge, about your measurement method. This will reduce the ”*black color*” of modern measurement instruments (if you do calculations offline…).
- Measurements can be modelled with respect to uncertainties before they are applied:
  -is the method *fit-for-purpose*?
  Meaning: Can we, or the customer, use the result for its intended for? (remember: the decision making)
- Which is the most effective way to go if there is a need for lower uncertainties?
  -*Longer measurement time?*
  -New calibration?
  -New equipment?,
  -A different method? (gamma spec vs. alpha spec vs. mass spec for e.g. long lived alpha emitters)
- Accreditation➔You have to do it! (Even if simple acceptance is used as the decision rule…)

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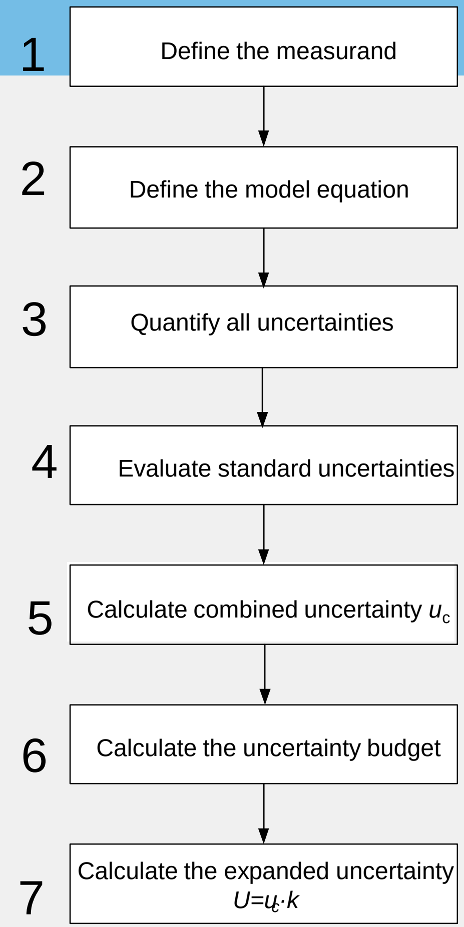
The GUM method:



+8: Reporting the measurement result

The GUM method

- **1: Define the measurand:**
  What is to be measured?
  Example: the activity of ^{137}Cs per mass of sample [Bq/kg]
- **2: The model equation:** $y = f(x_1, x_2, \ldots, x_n)$ a representation of $Y=f(X_1,X_2,\ldots,X_n)$
  The equation for calculation of the estimate of the measurand. It is a function of a number of input quantities. In many cases you already have the model equation if you extract raw data from your instrument and do all calculations 'off-line'!
  It is most often implemented in softwares for evaluation. However, a good practice is to **always** check the calculation done by the software…
- **3: Quantify all uncertainties:**
  -***Type A evaluation:***
  From statistics: *experimental standard deviation* or *experimental standard deviation of the mean* from repeated measurements
  -***Type B evaluation:*** Any other evaluation:
  From certificates, data bases, scientific judgement/previous knowledge,…

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The GUM method

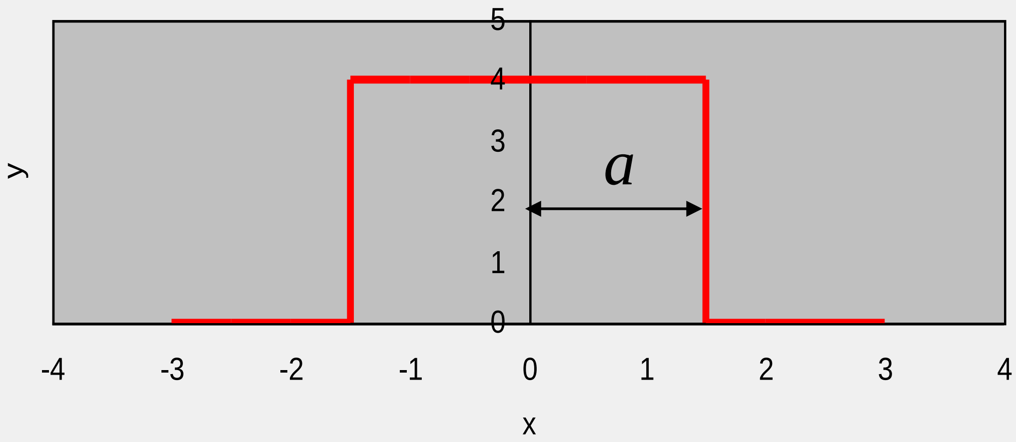
4: Evaluate standard uncertainties:

- Straight forward for Type A evaluations: Statistical evaluation of repeated observations
- Type B evaluations:
  Information from *e.g*. certificates? Is it a normal distribution? If not known, what do we do?
  Assumptions:
  -Rectangular distribution? *What is the standard unc?*
  -Triangular distribution? *What is the standard unc?*
  -Normal distribution? *What is the standard unc?*
  -…
- Assumptions?➔The uncertainty budget tells you if you need to reconsider, or *improve* your, assumption!

Rectangular distribution

1. Rectangular distribution:

We know an interval where we expect the quantity to be within. Zero probability that it is outside that interval, and all values within the interval are equally probable.

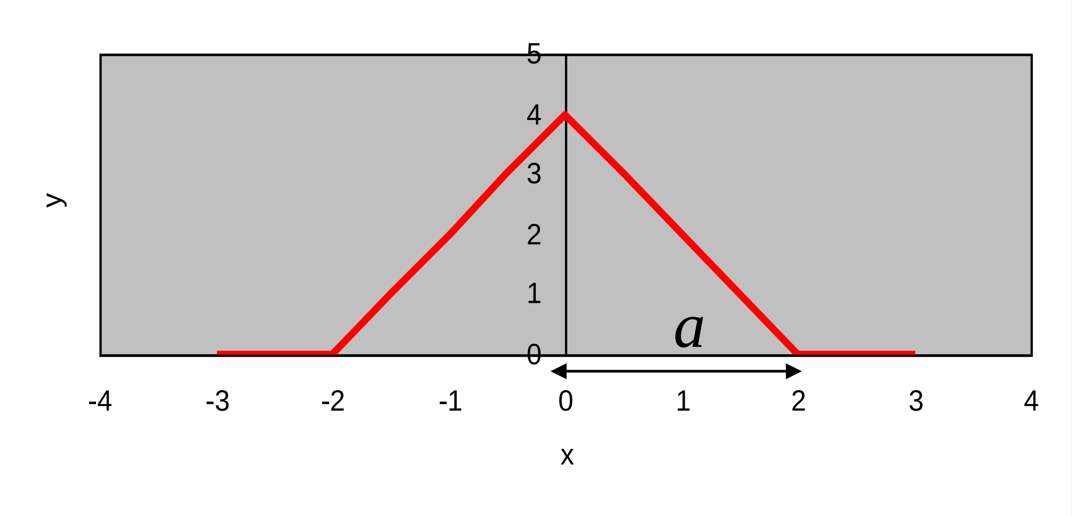


Standard unc: $$u = \frac{a}{\sqrt{3}}$$

Triangular distribution

2. Triangular distribution:

The mean value more probable
Probability of a value outside the interval is zero!

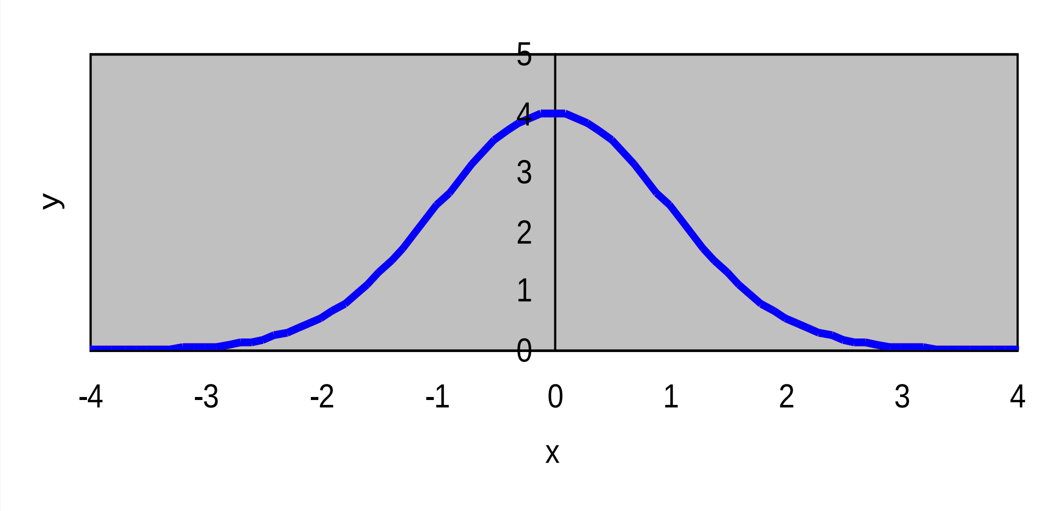


Standard unc: $$u = \frac{a}{\sqrt{6}}$$

Normal distribution

2. Normal distribution:

We get some clue:
-Standard uncertainty,
-coverage factor,
-confidence interval



$$k = 1 \Rightarrow 68\%$$

$$k = 2 \Rightarrow 95\%$$

Standard unc: $u = \dfrac{U}{k}$

The GUM method

5: Calculate the combined uncertainty:

- Uncertainty propagation (neglecting correlations):

$$u_y^{\,2} = \left(\frac{\partial y}{\partial x_1}\right)^2 \cdot u_{x1}^{\,2} + \left(\frac{\partial y}{\partial x_2}\right)^2 \cdot u_{x2}^{\,2} + \ldots + \left(\frac{\partial y}{\partial x_n}\right)^2 \cdot u_{xn}^{\,2} =$$

$$= \sum \left(\frac{\partial y}{\partial x_i}\right)^2 \cdot u_{xi}^{\,2}$$

- But we (most of us!) do not want to calculate partial derivatives (A model equation can be very long and complicated)…
- A need of a more useful expression
- For quick calculations: For ”simple” model equations where only multiplications and/or divisions are considered one can propagate relative uncertainties of the input quantities to get the relative uncertainty of the measurand.

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The GUM method

Uncertainty propagation on a computer without partial derivatives:

Definition of the derivative: $$\frac{\partial f}{\partial x_i} = \frac{f(x_i + h) - f(x_i)}{h} \quad \text{when } h \to 0$$

$$h = u(x_i) \Rightarrow u_c^2(y) \approx \sum \left(\frac{f(x_i + u(x_i)) - f(x_i)}{u(x_i)} \right)^2 \cdot \left(u(x_i)\right)^2$$

u should not be too large…

$$\Rightarrow \quad u_c^2(y) = \sum \left(f(x_i + u(x_i)) - f(x_i) \right)^2$$

The GUM method

- **6: Calculate the uncertainty budget:**
  -The contribution from each input quantity to the total variance:

$$\text{Variance contribution from parameter } i = \frac{\left(f(x_i + u(x_i)) - f(x_i)\right)^2}{\sum\left(f(x_i + u(x_i)) - f(x_i)\right)^2}$$

- Important tool if the uncertainty has to be reduced:
  -Uncertainty limited by counting statistics: *longer measurements; reduced background*; or limited by the calibration: *standard with lower stated uncertainty (lower uncertainty in the calibration),*…

The GUM method

- **7: Calculate the expanded uncertainty:**
  One standard uncertainty refers to about a 68% confidence interval. When reporting, the result should be given for an interval where we to a higher degree of confidence should expect the result to be within
- Most often a 95% confidence interval is used:

$$U = k \cdot u$$

- Then *k*=2 (approximately)!
- *k*: the coverage factor
- *k=2* results in fact of a 95.45% confidence interval. For a 95% confidence interval *k*=1.96
- All assuming normal distribution

The GUM method

- **8: Reporting the measurement result:**
  Most important: BE CLEAR!
  Remember: the measurement result is to be used for decision making!

- **Exemples on reporting[#] (expanded uncertainty):**

  -"*A*=40.2 Bq/kg with an expanded uncertainty *U*=3.0 Bq/kg calculated with a coverage factor *k*=2, resulting in an approximate confidence interval of 95%."

  -"*A*=40.2(30) Bq/kg, where the number within the paranthesis is an expanded uncertainty *U* calculated with a coverage factor of 2, i.e. corresponding to an approximate confidence interval of about 95%."

  - "*A*=(40.2±3.0) Bq/kg, where the number after ± is an expanded uncertainty *U* calculated with a coverage factor *k*=2 which corresponds to an approximate confidence interval of 95%."

[#] *Check ISO 17025 7.8.2 for additional reporting requirements!*

The model equation for gamma spectrometry

The model equation

The measurand A [Bq/kg] is calculated from the model equation. In gamma spectrometry the following model equation often holds:

$$A = \frac{N_{net}}{t_m \cdot \varepsilon \cdot k_{ET} \cdot I_\gamma \cdot m_{sample}} \cdot k_{TCS}$$

where

N_{net}: net number of counts
t_m: the measurement time
ε: measurement efficiency
k_{ET}: correction for geometry and matrix deviation
I_γ: photon emission probability
m_{sample}: mass of sample
k_{TCS}: correction for true coincidence summing (=1 for ^{137}Cs since no TCS)

How to evaluate standard uncertainties of the input quantities?

Examples of how the different uncertainties can be evaluated:

- Instrument signal: counting statistics
- Measurement time: uncertainty can (most often) be neglected
- Calibration: uncertainties of activites stated on certificates for *e.g.* the radionuclide solution used for the calibration. Often stated for k=2 (or 95% CI).
- Fit of efficiency function: Given by the software? (Not explicitly stated in the given model equation but can be included in the uncertainty of the efficiency.)
- Reproducability of the geometry: Perform a number (>10) of repeated measurements with the same 'sample'. Between every measurement the sample is replaced on the detector in the measurement position. Evaluate the standard deviation. Counting statistics has to be good (uncertainty<1%)… (Not explicitly stated in the model equation but can be included in the efficiency.)
- Photon emission probability: Databases (DDEP!). Observe: data in DDEP are given for k=1!
  Not all radionuclides are in DDEP…
- TCS: For 'well known' decay schemes the uncertainty may often be neglected
  (Shown at least for ^{134}Cs using a full Monte Carlo simulations of the geometry, detector and decay scheme: u_{TCS}<1%, k=1.)
- k_{ET}: MC may be one tool. Sensitivity analysis another. Largest problem? for solid samples, difficult to get a flat uniform surface, and for low energies measuring *e.g*. sediment samples with unknown composition.
  What is the limits for k_{ET}? Max-min k_{ET} and applying a rectangular distribution might be one way.
- Sub-sampling of particulate samples… Not covered here

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Calculating combined uncertainties

Different tools:

- **Partial derivatives:**
  -The hard way!
- **Dedicated softwares…**
- **Monte Carlo (MC) methods (covered on Thursday):**
  -When no analytical solution to the model equation can be stated (in gamma ray spectrometry this is not the case)
  -MC-methods handle all kinds of distributions as well as non-linearities. Results in an empirical pdf.
- **A spreadsheet model according to Kragten**

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Kragten spreadsheet

- Uncertainty propagation is easily implemented as a spreadsheet model
- Remember (or better: use a cheat sheet) only two things:

$$u_c^{\,2}(y) = \sum \left(f(x_i + u(x_i)) - f(x_i) \right)^2$$

$$\text{Variance contribution from parameter } i = \frac{\left(f(x_i + u(x_i)) - f(x_i) \right)^2}{\sum \left(f(x_i + u(x_i)) - f(x_i) \right)^2}$$

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Kragten spreadsheet (a systematic scheme for uncertainty propagation)

Input quantities:	a	b	c	d
	u(a)	**u(b)**	**u(c)**	**u(d)**
=a	**=a+u(a)**	=a	=a	=d
=b	=b	**=b+u(b)**	=b	=b
=c	=c	=c	**=c+u(c)**	=c
=d	=d	=d	=d	**=d+u(d)**
=f=f(a,b,c,d)	=f(a+u(a),b,c,d)	=f(a,b+u(b),c,d)	=f(a,b,c+u(c),d)	=f(a,b,c,d+u(d))
Differenser=	=f-f(a+u(a),b,c,d)	=f-f(a,b+u(b),c,d)	=f-f(a,b,c+u(c),d)	=f-f(a,b,c,d+u(d))
Diff^2=	=(f-f(a+u(a),b,c,d))^2	=(f-f(a,b+u(b),c,d))^2	=(f-f(a,b,c+u(c),d))^2	=(f-f(a,b,c,d+u(d))^2

uc^2= **=SUM(Diff^2)**

$$u_c^2(y) = \sum \left(f(x_i + u(x_i)) - f(x_i) \right)^2$$

uc= **=SQRT(SUM(Diff^2))**

Uc= **=k·uc**

or -. Why?

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An example

^{137}Cs was measured. Data for the measurement was:

N_{net}=5640±90

t_m=4 h=14400 s (constant)

I_γ=0.8499±0.0020 (differ now!)

ε=0.0150±0.0003

k_{ET}=1.000±0.0020

m_{sample}=0.06000±0.00006

k_{TCS}=1.00 (no uncertainty since no TCS)

All data for *k*=1.

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The example

$$A = \frac{N_{net}}{t_m \cdot \varepsilon \cdot k_{ET} \cdot I_\gamma \cdot m_{sample}} \cdot k_{TCS}$$

N_net	5640	
t_m	14400	s
I_g	0.8499	
ε	0.015	
k_ET	1	
m_sample	0.06	kg
k_TCS	1	

A = 512.0428 Bq/kg

	N_net	t_m	I_g	ε	k_ET	m_sample	k_TCS
u_i=	90	0	0.002	0.0003	0.02	0.00006	0
	5730	5640	5640	5640	5640	5640	5640
	14400	14400	14400	14400	14400	14400	14400
	0.8499	0.8499	0.8519	0.8499	0.8499	0.8499	0.8499
	0.015	0.015	0.015	0.0153	0.015	0.015	0.015
	1	1	1	1	1.02	1	1
	0.06	0.06	0.06	0.06	0.06	0.06006	0.06
	1	1	1	1	1	1	1
	520.2137	512.0428	510.8407	502.0028	502.0028	511.53128	512.0428
Diff=	8.170896	0	-1.20212	-10.0401	-10.0401	-0.5115313	0
Diff^2=	66.76354	0	1.445091	100.8027	100.8027	0.2616643	0
SumDiff^2=	270.0757						
Unc contribution (%)=	24.72	0	0.54	37.32	37.32	0.10	0

***u*_c=** 16.43398 Bq/kg

***k*=** 2

***A*=**	512	Bq/kg
***U*=**	33	Bq/kg
***U*_rel=**	6.4	%

Subtracting u_i in this example gives: A=(512±34) Bq/kg, k=2 (U_{rel}=6.6%)

The example

- Use this example as a ’template’ for you uncertainty calculations if you’re not already doing it
- Hopefully I have done the math correct, if not let me know!

A small cliffhanger:

Monte Carlo method(s)

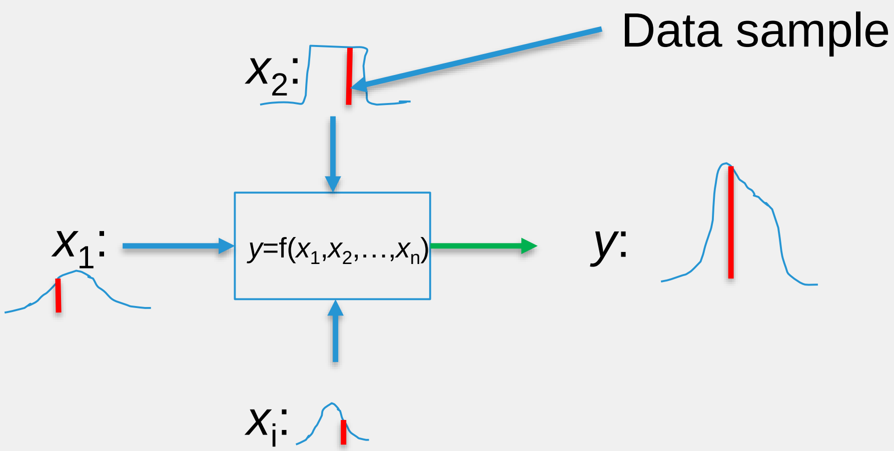
Will be covered more on Thursday

A general reference to MCM for uncertainty calculations

- *Evaluation of measurement data – Supplement 1 to the "Guide to the expression of uncertainty in measurement" – Propagation of distributions using a Monte Carlo method*, JCGM 101:2008

MC calculation: Principle

Propagation of distributions:



Data are drawn randomly from the PDFs of each input quantity
➔In ’brute force’ MC many data needed to ensure sampling from the tails of *e.g.* Gaussian PDF (where the probability is low).

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Three very nice guides

- JCGM 100:2008
  Evaluation of measurement data-Guide to the expression of uncertainty in measurement
- JCGM 101:2008
  Evaluation of measurement data-Supplement 1 to the ”Guide to the expression of uncertainty in measurement”-Propagation of distributions using a Monte Carlo method
- JCGM 106:2012
  Evaluation of measurement data-The role of measurement uncertainty in conformity assessment

Thank you!

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