Approaches to measurement uncertainty evaluation

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Science
for a safer world

Introduction

- Basic principles – a reminder
- Uncertainty from a measurement equation
- Gradient methods
  - Finite difference approach
  - Kragten's method
- Simulation methods
  - Monte Carlo simulation (MCS)

Measurement uncertainty: Basic principles

Measurement uncertainty - ISO definition

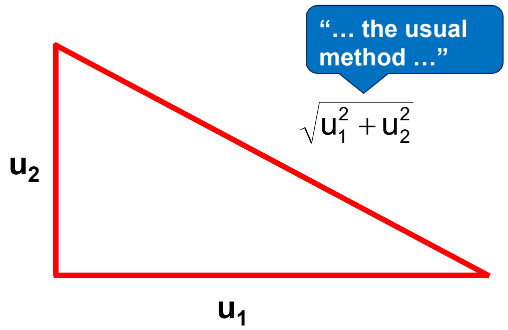
"A parameter, associated with the result of a measurement, that characterises the dispersion of the values that could reasonably be attributed to the measurand"

The part of the result after the ±

ISO recommendations

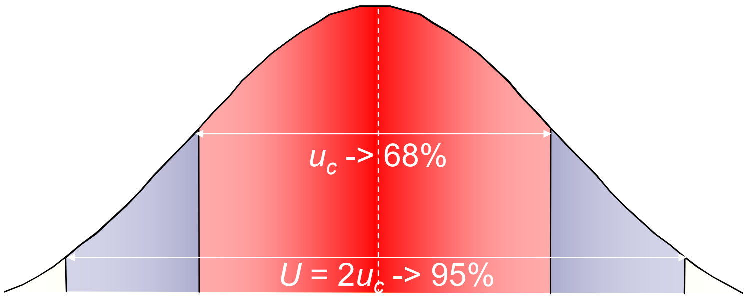
- Uncertainties arise from several contributions
- Two ways of evaluating uncertainty components
  - statistical (Type A) and otherwise (Type B)
  - should be treated in the same way
- Expression as standard deviations
- Combination by ".. the usual method for the combination of variances."
- Multiplied by a (stated) factor if required

Implementation - combining uncertainties



- The uncertainties are:
  - Uncertainty contributions for the same quantity
  - In the same units
  - Expressed as 'standard uncertainties'

Expanded uncertainty *U*



$U = k.u_c$

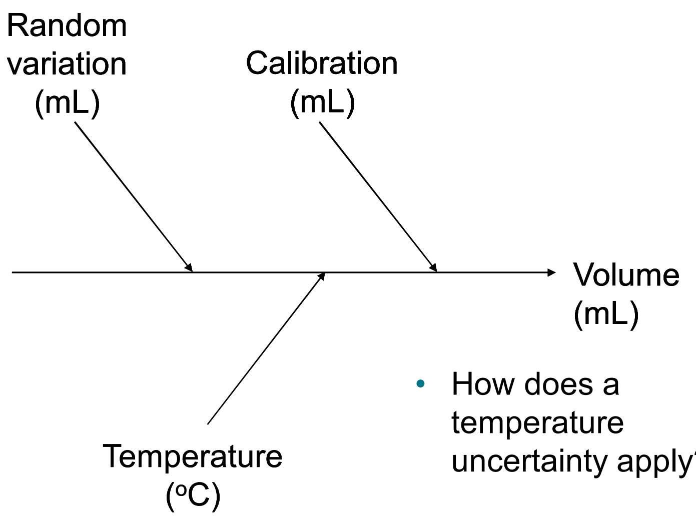
Uncertainties in different quantities: "Propagation of uncertainty"

Example: The effect of temperature on volume

Dispense 100ml
from a Calibrated volumetric flask (*U* = 0.2 ml, k=2)
allowing for random filling effects (*s* = 0.1 ml)
at a laboratory temperature 20 ± 2 °C

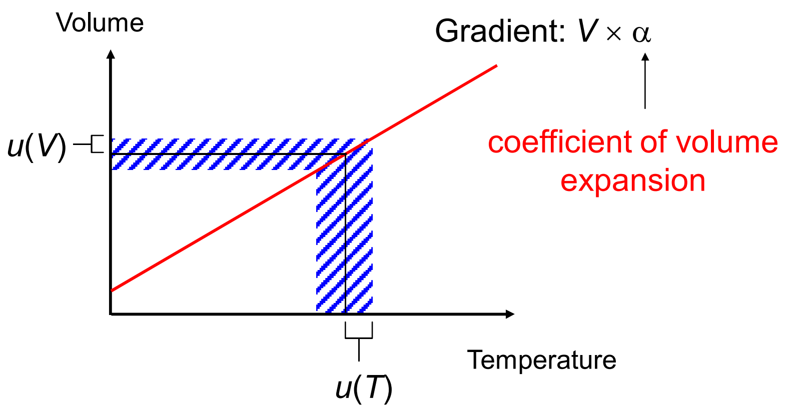
- Estimate the uncertainty in dispensed volume at 20 °C

Example: The effect of temperature on volume



- How does a temperature uncertainty apply?

Example: The effect of temperature on volume



$u(V)$ = gradient $\times$ $u(T)$

The 'law of propagation of uncertainty'

- x_i parameter affecting analytical result y
- $u(x_i)$ uncertainty in x_i
- $u_i(y)$ uncertainty in y due to uncertainty in x_i

$$u_i(y) = \sqrt{\sum_i \left(\frac{\partial y}{\partial x_i}\right)^2 u(x_i)^2}$$

sensitivity coefficient

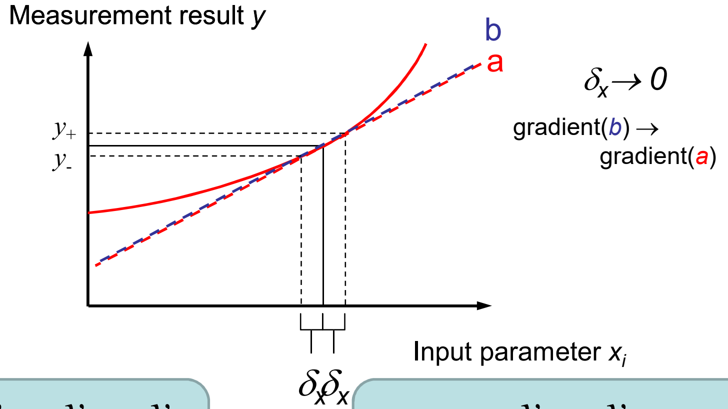
Describes how much the result changes with changes in input

Numerical methods for uncertainty propagation

Why include numerical methods?

- Simpler than algebra
- More general than algebraic differentiation
  - Can obtain gradients when differentiation is intractable
    - Result obtained from algorithm rather than equation
  - May be applicable when simplifying assumptions do not apply
    - Uncertainties large
    - $f(\ldots)$ not linear
    - Distributions far from Normal

Finite difference - principle



$$\frac{\partial y}{\partial x_i} \approx \frac{y_+ - y_-}{2\delta_{x_i}}$$

$$u_i(y) \approx \frac{y_+ - y_-}{2\delta_{x_i}} u(x_i)$$

Compare finite difference with the GUM

GUM first order

Expression: a/(b - c)

Uncertainty budget:

	x	u	c	u.c
a	1	0.05	1	0.05
b	3	0.15	-1	-0.15
c	2	0.10	1	0.10

y: 1
u(y): 0.1870829

Finite Difference

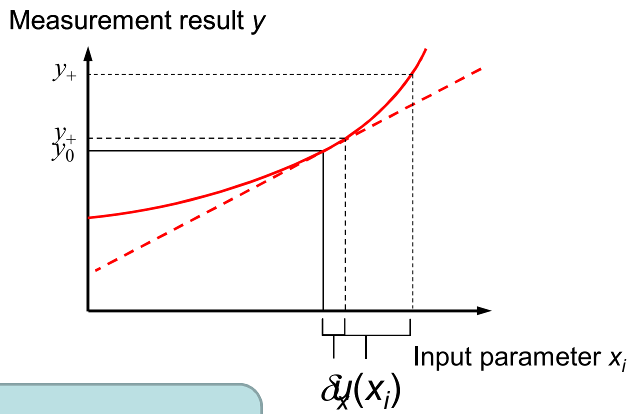
Expression: a/(b - c)

Uncertainty budget:

	x	u	c	u.c
a	1	0.05	1.000000	0.0500000
b	3	0.15	-1.000002	-0.1500003
c	2	0.10	1.000001	0.1000001

y: 1
u(y): 0.1870832

Kragten's method



$$u_i(y) \approx y_+ - y_0$$

Eurachem guide, sec E.2

Compare Kragten with FD

Finite Difference

Expression: a/(b - c)

Uncertainty budget:

	x	u	c	u.c
a	1	0.05	1.000000	0.0500000
b	3	0.15	-1.000002	-0.1500003
c	2	0.10	1.000001	0.1000001

y: 1
u(y): 0.1870832

Kragten

Expression: a/(b - c)

Uncertainty budget:

	x	u	c	u.c
a	1	0.05	1.0000	0.05000
b	3	0.15	-0.8695	-0.13043
c	2	0.10	1.1111	0.11111

y: 1
u(y): 0.1784906

Exact vs. Numerical

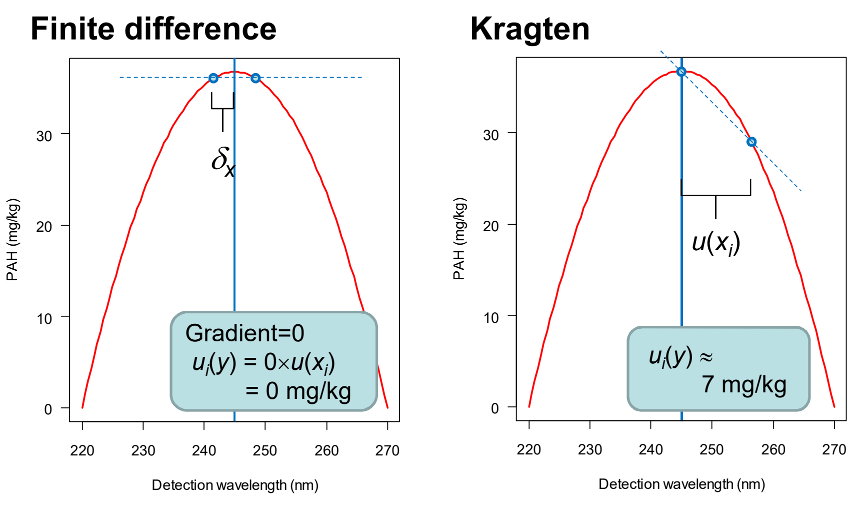
$y = a/(b - c)$

Uncertainties:

	x	u
a	1	0.05
b	3	0.15
c	2	0.10

Method	Standard uncertainty
'Exact' first order (GUM)	0.1870829
Finite difference (0.01u)	0.1870832
Kragten	0.1784906

Why use a 'less accurate' method?



Finite difference methods compared

Finite difference 1st order

- Accurate gradient
- Faithfully reproduces 1st order GUM uncertainty
- Simple to calculate

- 1st order GUM is insufficient for highly non-linear cases
  - Needs 2nd and higher order

Kragten

- Exact only for linear examples
- Does not reproduce 1st order GUM
- Simple to calculate

- Usually adequate for mild nonlinearity
- May be **better** for highly non-linear cases

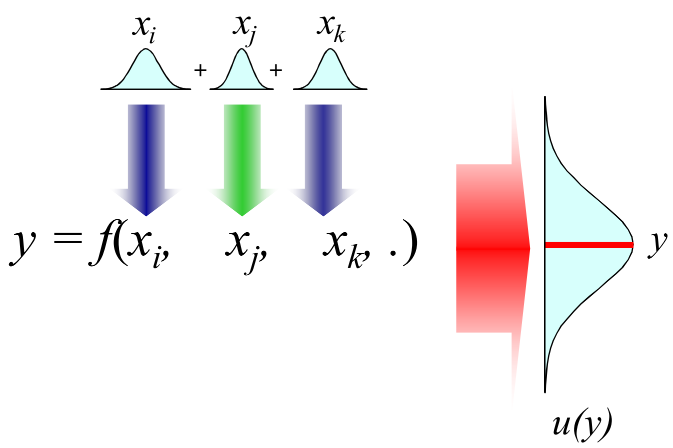
Both much simpler than manual differentiation

Monte Carlo/simulation methods

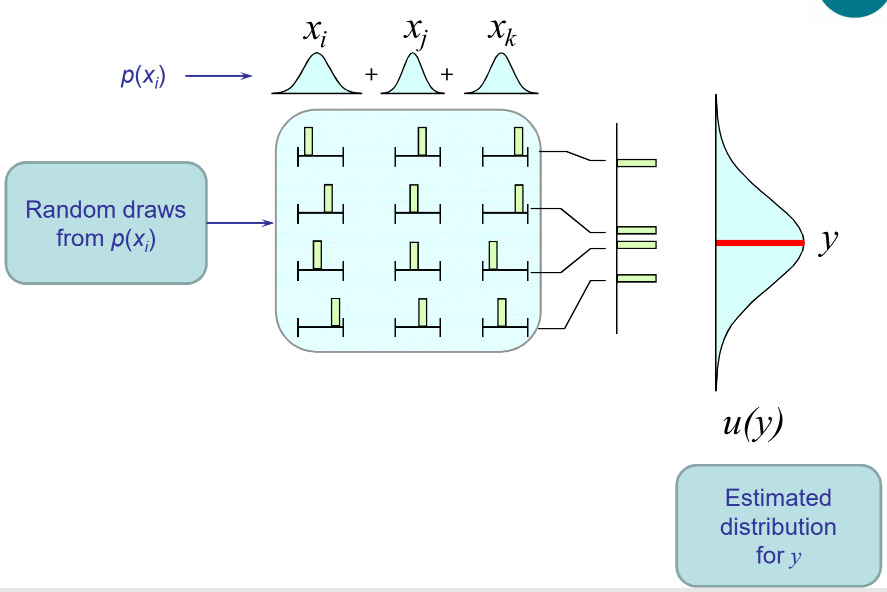
GUM Supplement 1 (JCGM 101)

Eurachem guide: QUAM:2012

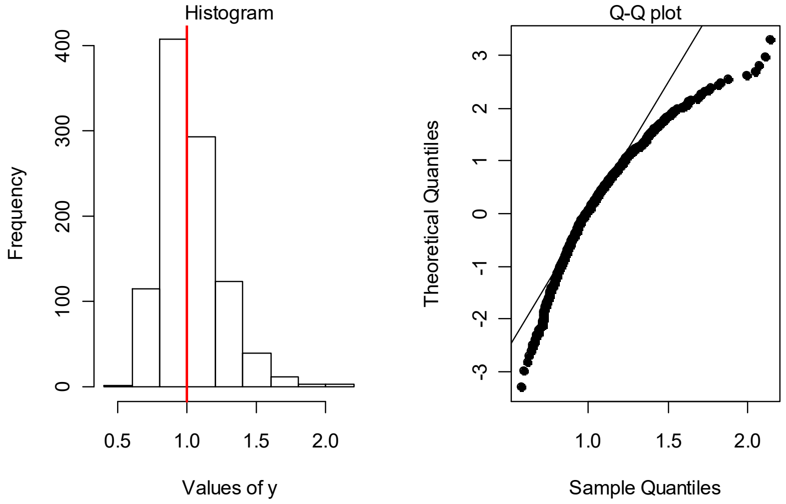
Principle of simulation
i) The problem



Principle of simulation



MCS example
y = *a*/(*b*-*c*) (999 replicates)



Calculations carried out using metRology 0.9-24 (http://sourceforge.net/projects/metrology/)

Exact vs. Numerical

y = *a*/(*b* - *c*)

Uncertainties:

	x	u
a	1	0.05
b	3	0.15
c	2	0.10

Method	Standard uncertainty
'Exact' first order (GUM)	0.1870829
Finite difference (0.01u)	0.1870832
Kragten	0.1784906
MCS	0.221 *y* = 0.718 to 1.535 *-0.3; +0.5*

Summary

- Numerical methods work
  - when used with care
- Finite difference and Kragten methods are simple to calculate and usually reliable
  - Kragten's method less like 1st order – but this is often good!
- Simulation methods show **distributions**
  - Applicable to non-normal cases
- MCS (JCGM 101) simple in principle but computer intensive
- Future guidance will include further methods
  - Notably Bayesian approaches

Software

- Simple algebraic, Kragten, Finite Difference and MCS
  - metRology version 0.9-4 running under R
    http://sourceforge.net/projects/metrology