Numerical methods for uncertainty evaluation
An overview

S L R Ellison
LGC Limited, Teddington, UK

Introduction

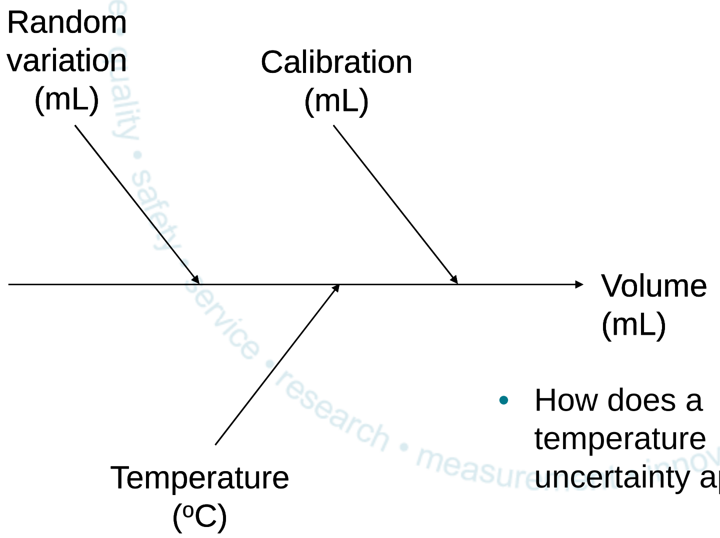
- Uncertainty from a measurement equation
- Gradient methods
  - Finite difference approach
  - Kragten's method
- Simulation methods
  - Monte Carlo simulation (MCS)
  - Bayesian approach using Markov chain Monte Carlo (MCMC)

A volumetric example

- 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

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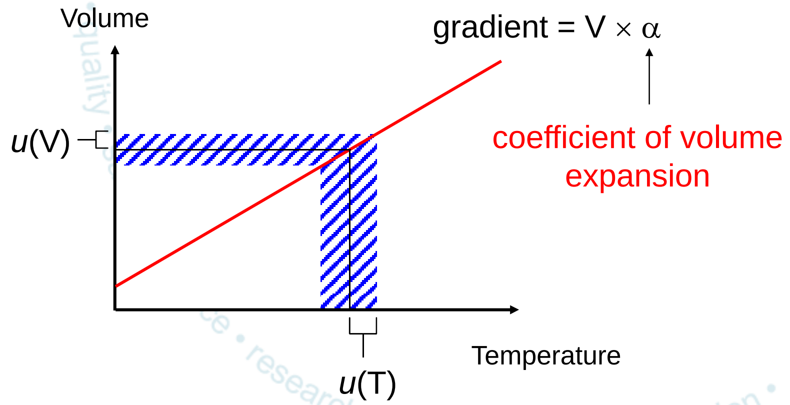

$u(V) = \text{gradient} \times u(T)$

Uncertainty propagation

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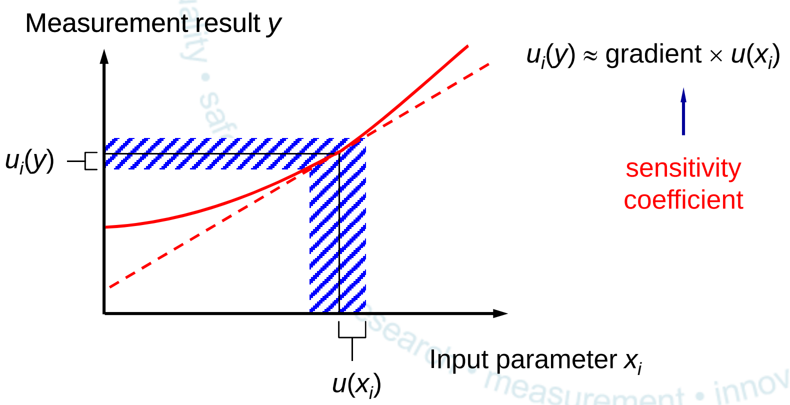


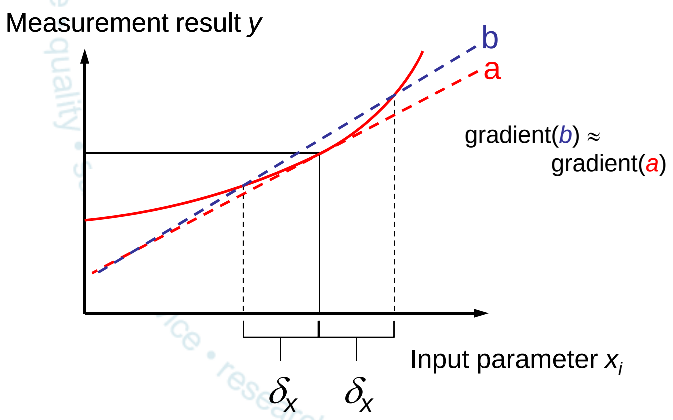
Mathematical form of uncertainty

- 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

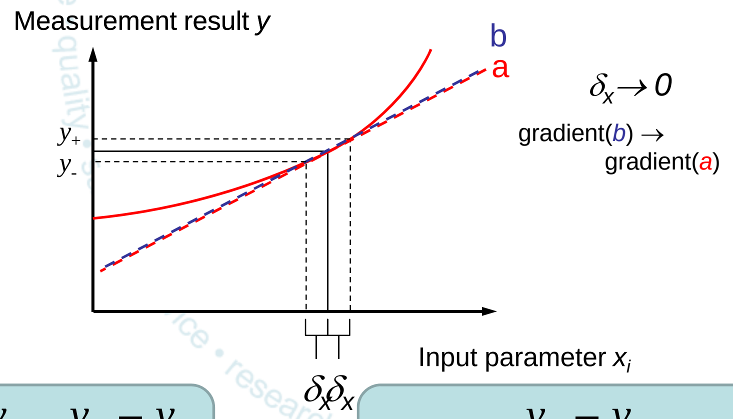
$$u_i(y) = \sqrt{\sum_i \left(\frac{\partial y}{\partial x_i}\right)^2 u(x_i)^2}$$

↑ sensitivity coefficient

Finite difference method



Finite difference method



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

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

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

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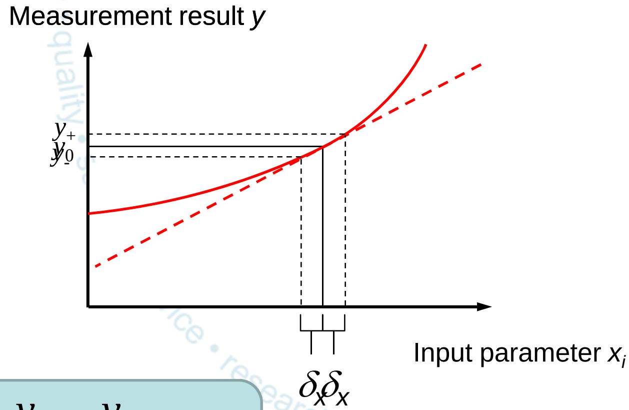

$$u_i(y) \approx \frac{y_+ - y_0}{\delta_{x_i}} u(x_i)$$

Kragten's method

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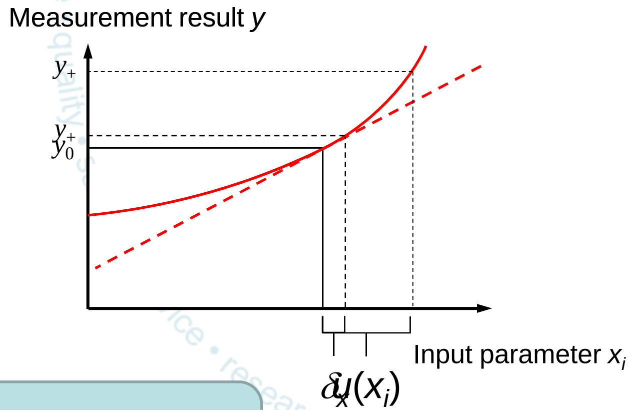

$$u_i(y) \approx y_+ - y_0$$

Compare Kragten with FD

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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

Why use a ‘less accurate’ method?

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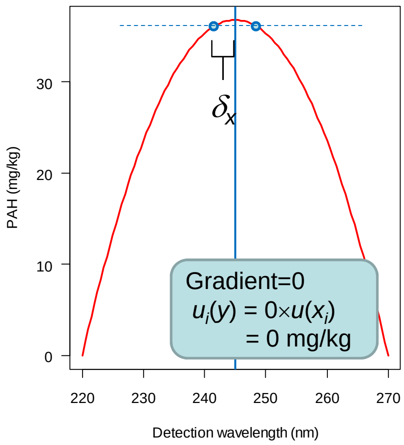
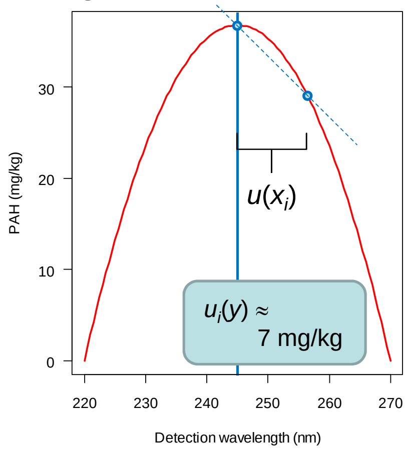
Finite difference



Kragten



Finite difference methods compared

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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

Principle of simulation

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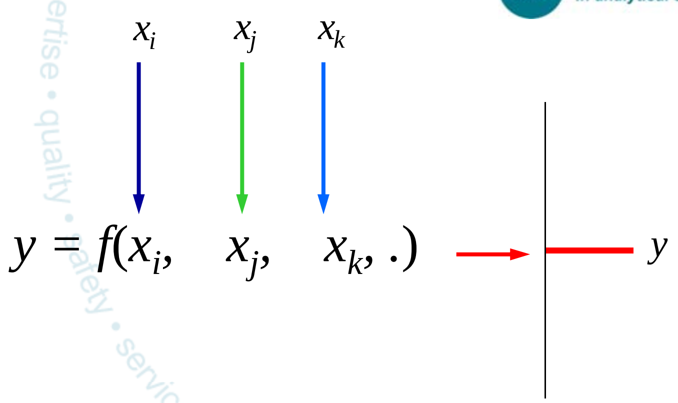

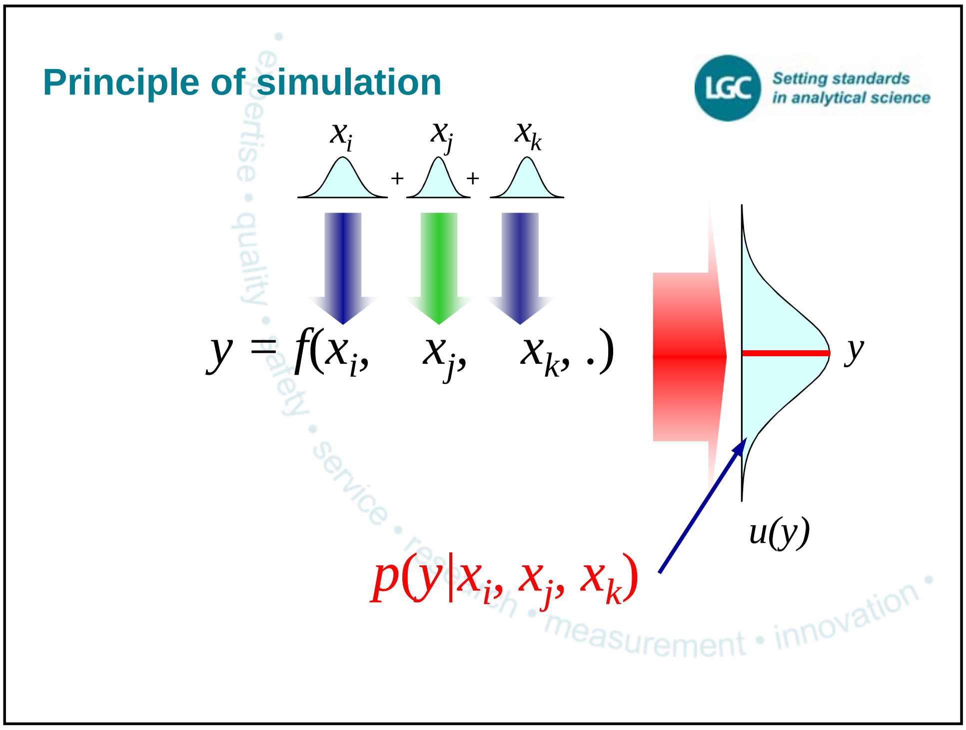
Principle of simulation
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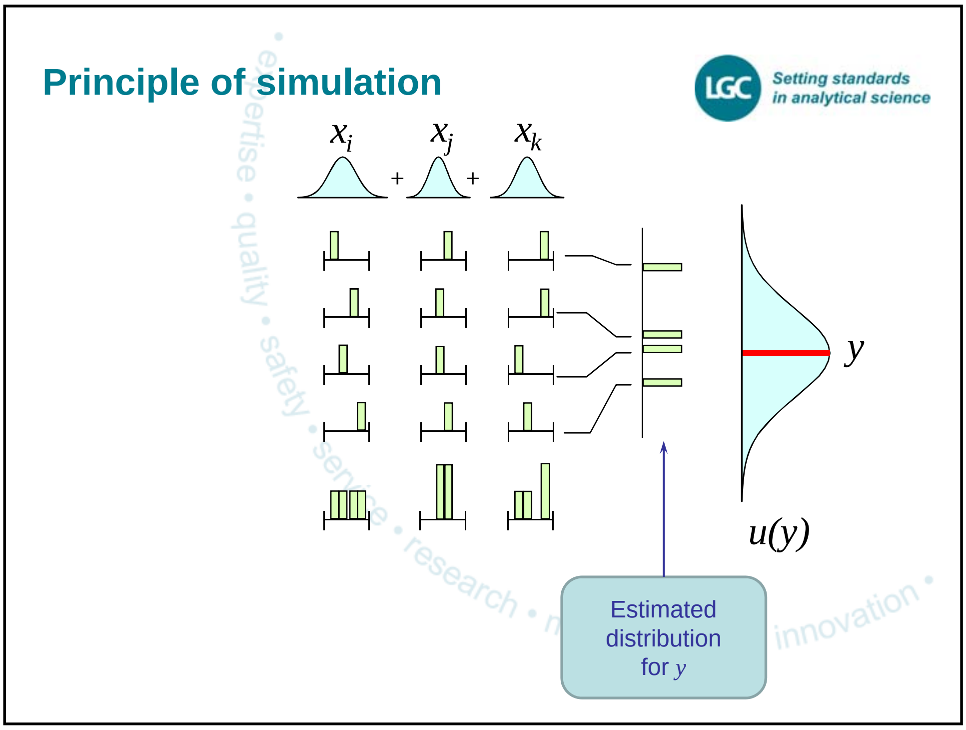
x_i
x_j
x_k
+
+
$y = f(x_i, \quad x_j, \quad x_k, .)$
y
$u(y)$
$p(y|x_i, x_j, x_k)$


Principle of simulation
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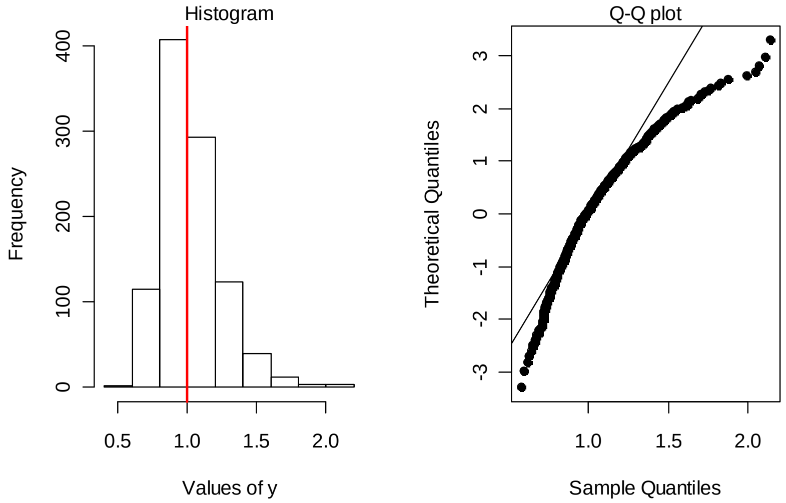
x_i
x_j
x_k
+
+
y
$u(y)$
Estimated distribution for y

GUM Supplement 1 ‘Propagation of distributions’ using MCS

- Starts from observed *x* and *u*
- Assumes distributions appropriate to input quantities
- Samples from each (“Monte Carlo simulation”)
  - calculates *y* for each sample
- Calculates *u*(*y*) from ‘observed’ distribution
- Can calculate quantiles to provide coverage interval
  - May be asymmetric
- Only corresponds to distribution for the true value under some assumptions

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



Calculations carried out using metRology 0.9-4 (http://sourceforge.net/projects/metrology/)

Compare GUM and MCS

GUM

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

y = 1 ± 0.37 (*k*=2)

MCS

Expression: a/(b - c)

Uncertainty budget:

	x	u	c	u.c
a	1	0.05	1.08	0.054
b	3	0.15	-1.09	-0.16
c	2	0.10	1.06	0.11

y: 1

u(y): 0.221

y = 0.718 to 1.535

Bayesian estimate using Markov Chain MC

MCS (Supplement 1)

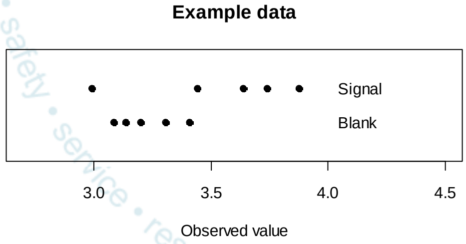
- Samples from distributions for input quantities
- Calculates *y*
- Generates a distribution for the value of the measurand if
  - Distribution of *x* does not depend on *y*
  - There are no prior constraints on *y*

Bayes/MCMC

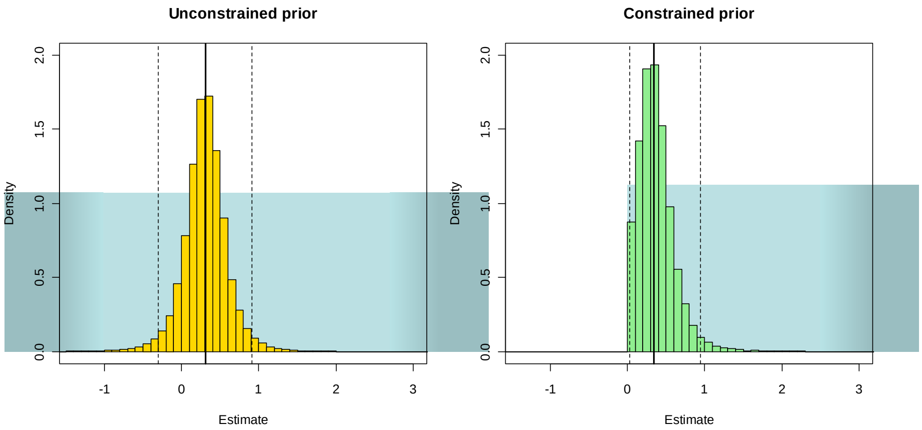
- Starts from assumed distribution for *y*
- Produces samples which reflect ‘likelihood’ of *y* given data *x*
- Always generates *a* distribution for the value of the measurand
- Depends somewhat on choice of prior

MCMC example

- *y* is a concentration calculated from a signal minus a blank value



MCMC example - results



Uniform priors assumed for *y* and for both variances; error distributions assumed normal.

Calculations carried out using WinBUGS 1.4

Summary

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- 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
  - Not just standard uncertainties
- MCS (GS1) simple but computer intensive
- MCMC more appropriate for constraints and *x* distribution dependent on *y* (eg proportional sd)
  - but much more difficult – specialist software only

Software

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- Simple MCS, Kragten and Finite Difference
  - metRology version 0.9-4 running under R version 2.12
  - http://sourceforge.net/projects/metrology
- Bayesian MCMC calculation
  - WinBUGS version 1.4.3
  - http://www.mrc-bsu.cam.ac.uk/bugs/winbugs/contents.shtml