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 $20 \pm 2$ °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

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

Uncertainty propagation

\[ u(y) \approx \text{gradient} \times u(x_i) \]
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 $x_i$

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

Finite difference method

Measurement result $y$

Input parameter $x_i$

gradient(b) \approx gradient(a)
Finite difference method

\[ \frac{\partial y}{\partial x_i} \approx \frac{y_+ - y_-}{2\delta x_i} \]

\[ \delta y \approx \frac{y_+ - y_-}{2\delta x_i} \]

\[ y \approx y_0 + \delta y \]

\[ u_i(y) \approx \frac{y_+ - y_-}{2\delta x_i} u(x_i) \]

Compare finite difference with the GUM

GUM first order
Expression: \( a/(b - c) \)

Uncertainty budget:

<table>
<thead>
<tr>
<th></th>
<th>( x )</th>
<th>( u )</th>
<th>( c )</th>
<th>( u.c )</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>1</td>
<td>0.05</td>
<td>1</td>
<td>0.05</td>
</tr>
<tr>
<td>b</td>
<td>3</td>
<td>0.15</td>
<td>-1</td>
<td>-0.15</td>
</tr>
<tr>
<td>c</td>
<td>2</td>
<td>0.10</td>
<td>1</td>
<td>0.10</td>
</tr>
</tbody>
</table>

Finite Difference
Expression: \( a/(b - c) \)

Uncertainty budget:

<table>
<thead>
<tr>
<th></th>
<th>( x )</th>
<th>( u )</th>
<th>( c )</th>
<th>( u.c )</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>1</td>
<td>0.05</td>
<td>1.000000</td>
<td>0.0500000</td>
</tr>
<tr>
<td>b</td>
<td>3</td>
<td>0.15</td>
<td>-1.000002</td>
<td>-0.1500003</td>
</tr>
<tr>
<td>c</td>
<td>2</td>
<td>0.10</td>
<td>1.000001</td>
<td>0.1000001</td>
</tr>
</tbody>
</table>

\( y: 1 \)
\( u(y): 0.1870829 \)

\( y: 1 \)
\( u(y): 0.1870832 \)
Kragten’s method

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

\[ u_i(y) \approx y_+ - y_0 \]
Compare Kragten with FD

Finite Difference
Expression: \( a/(b - c) \)

Uncertainty budget:

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>1</td>
<td>0.05</td>
<td>1.000000</td>
</tr>
<tr>
<td>b</td>
<td>3</td>
<td>0.15</td>
<td>-1.000002</td>
</tr>
<tr>
<td>c</td>
<td>2</td>
<td>0.10</td>
<td>1.000001</td>
</tr>
</tbody>
</table>

Kragten
Expression: \( a/(b - c) \)

Uncertainty budget:

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>1</td>
<td>0.05</td>
<td>1.0000</td>
</tr>
<tr>
<td>b</td>
<td>3</td>
<td>0.15</td>
<td>-0.8695</td>
</tr>
<tr>
<td>c</td>
<td>2</td>
<td>0.10</td>
<td>1.1111</td>
</tr>
</tbody>
</table>

Why use a ‘less accurate’ method?

Finite difference

Gradient=0
\( u(y) = 0 \times u(x_i) = 0 \text{ mg/kg} \)

Kragten

\( u(y) \approx 7 \text{ mg/kg} \)
Finite difference methods compared

Finite difference 1\textsuperscript{st} order
- Accurate gradient
- Faithfully reproduces 1\textsuperscript{st} order GUM uncertainty
- Simple to calculate
- 1\textsuperscript{st} order GUM is insufficient for highly non-linear cases
  - Needs 2\textsuperscript{nd} and higher order

Kragten
- Exact only for linear examples
- Does not reproduce 1\textsuperscript{st} 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

\[ y = f(x_i, x_j, x_k, \ldots) \]

- \( x_i \)
- \( x_j \)
- \( x_k \)
- \( y \)
Principle of simulation

\[
y = f(x_i, x_j, x_k, \ldots)
\]

\[
p(y|x_p, x_p, x_k)
\]

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

<table>
<thead>
<tr>
<th>GUM</th>
<th>MCS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Expression: a/(b - c)</td>
<td>Expression: a/(b - c)</td>
</tr>
</tbody>
</table>

Uncertainty budget:

<table>
<thead>
<tr>
<th></th>
<th>x</th>
<th>u.c</th>
<th>u.c</th>
<th></th>
<th>x</th>
<th>u.c</th>
<th>u.c</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>1</td>
<td>0.05</td>
<td>0.05</td>
<td>a</td>
<td>1</td>
<td>0.05</td>
<td>1.08</td>
</tr>
<tr>
<td>b</td>
<td>3</td>
<td>0.15</td>
<td>-1</td>
<td>-0.15</td>
<td>b</td>
<td>3</td>
<td>0.15</td>
</tr>
<tr>
<td>c</td>
<td>2</td>
<td>0.10</td>
<td>1</td>
<td>0.10</td>
<td>c</td>
<td>2</td>
<td>0.10</td>
</tr>
</tbody>
</table>

\[ y = 1 \pm 0.37 \quad (k=2) \]
\[ y = 1 \pm 0.37 \quad (k=2) \]

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

Example data

Example data

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

Example data

MCMC example - results

MCMC example - results

Unconstrained prior

Constrained prior

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

Calculations carried out using WinBUGS 1.4
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
  – 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

• 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