Future directions in measurement uncertainty evaluation

S L R Ellison
LGC Limited, Teddington, UK

Science
for a safer world

Introduction

• Existing approaches – a reminder

• A Bayesian approach to uncertainty evaluation

• Future guidance from JCGM
‘Law of propagation of uncertainty’ (LPU)

- Current GUM approach

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

- Limitations
  - Simple form assumes symmetry, small uncertainties, approximate linearity
  - Relies on simple form for y (must be differentiable)
  - Extensions allow for correlation, non-linearity etc

Monte Carlo simulation (MCS)

- GUM Supplement 1
- Does not require differentiable form for y
- Allows for asymmetry, non-linearity
- Does not cope with constraints on y
Handling constraints on $y$: Bayesian methods

Bayes Theorem

- Probability after a measurement depends on
  - The probability before the measurement
  - The ‘strength’ of evidence from the measurement

\[
P(A|M) = P(A) \frac{P(M|A)}{P(M)}
\]
Bayes applied to Measurement Uncertainty

Prior for $\mu$

Likelihood from $x$

Posterior for $\mu$

i) The mean shifts

ii) The distribution differs
### Bayesian estimate using Markov Chain MC

**MCS (Supplement 1)**
- Samples from distributions for input quantities \( x \)
- 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 \( \mu \)
- 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

### Bayes and measurement uncertainty: Avoiding controversy

**Rule 1**: The default: Use an uninformative prior
  - Typically wide Normal or Uniform

**Rule 2**: There are no truly uninformative priors
  - And some 'uninformative' priors can be unexpectedly informative

**Rule 3**: If an uninformative prior works for measurement uncertainty, there’s probably an easier way

*Bayes theorem is most useful for uncontroversial, informative priors*
Bayes via Markov Chain Monte Carlo (MCMC)

- Simulate from 'Proposal' for $\mu$
- "Filter" through Likelihood
- Posterior for $\mu$
- Base next point on previous accepted point

MCMC example

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

Example data

- True concentration cannot be below zero
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

MCMC example 2:
Dispersion proportional to \( \mu \)

Example data

- Concentration: not below zero
- Common observation: standard deviation proportional to true value
MCMC results:
i) Fixed standard deviation

\[ \mu \text{ (fixed sigma)} \]

Density

-0.5 0.0 0.5 1.0 1.5

0 1 2 3 4

\[ \sigma \propto \mu \]

MCMC results

ii) Proportional standard deviation

\[ \mu \text{ (proportional sigma)} \]

Density

\[ \sigma \propto \mu \]
The case for Bayesian methods

• Bayesian methods cope correctly with
  – Constraints on y
  – Distributions dependent on true value

• Bayes’ theorem answers the right question
  – MCS: “Where could my next result be, if my result is the true value?”
  – Bayes: “Where could the true value be if this is my data?”

• BUT: Bayes is hard
  – Much more difficult – specialist software only
  – Choosing a ‘prior distribution’ is not simple
  – Interpretation needs care

Future JCGM guidance
JCGM

• Joint Committee for Guides in Metrology
  – Formed in 1997
• Members are international metrology and standards bodies:
  – BIPM, OIML, ISO, IEC, IUPAC, IUPAP, IFCC, ILAC*
• Responsible for guides on
  – Measurement uncertainty (WG1)
  – Terminology (the VIM) – WG2

*ILAC joined in 2005

Existing JCGM guidance on MU

• JCGM 100:2008 Guide to the expression of Uncertainty in Measurement (“the GUM”)
• JCGM 101:2008 Supplement 1 to the “Guide to the expression of uncertainty in measurement” – Propagation of distributions using a Monte Carlo method
• JCGM 102:2011 Supplement 2 to the “Guide to the expression of uncertainty in measurement” – Extension to any number of output quantities
• JCGM 104: An introduction to the "Guide to the expression of uncertainty in measurement" and related documents
• JCGM 106:2012 The role of measurement uncertainty in conformity assessment
Draft GUM replacement

- Bayesian basis
  - Used Bayesian posterior mean and variance for input quantities
  - LPU for small uncertainties
  - MCS (Supplement 1) for non-linear cases etc

- Issued for public comment in late 2014
- Substantial adverse comment from member bodies
- Development suspended

JCGM new direction

- Guide to the expression of uncertainty in measurement
- Introduction based on JCGM 100:2008
- New introduction guiding choice
- Single title for complete suite
- "New" GUM included as option
- Current GUM JCW 100:2008
- Monte Carlo method JCW 101:2008
- Multivariate measurements JCW 102:2011
- Conformity assessment JCW 105:2012
- Modelling measurements JCW 106:2014
- Examples JCW 110
- LPU in a Bayesian framework JCW 111
- Interlaboratory comparisons JCW
- CIPM Key comparisons
- Current GUM retained
- Separate examples
- Concepts and principles JCW 105
- Least square methods JCW 101
- Bayesian methods JCW 106
- Formal Bayesian treatment
Summary

• JCGM see Bayesian reasoning as fundamental
• Existing guidance can be seen as special cases
  – GUM: Small uncertainties; Near normality; No ‘prior’ information
  – MCS: Non-normal distributions; No ‘prior’ information

• Future JCGM guidance is ‘modular’
  – Different treatments for different circumstances