New approaches to uncertainty evaluation:

Propagation of uncertainty, numerical methods and Monte Carlo simulation

Wolfram Bremser

BAM Federal Institute for Materials Research and Testing
Unter den Eichen 87, 12205 Berlin, Germany

Topics:

- Sources and principles
- Uncertainty propagation
- Numerical method („Kragten approach“)
- MC applied to uncertainty estimation
- Conclusions

Sources: ISO GUM and EURACHEM Guide

- **ISO/IEC Guide 98; Uncertainty of measurement**

  Part 3: Guide to the expression of uncertainty in measurement (GUM:1995) → **MU propagation**

  Guide 98-3/Suppl 1:2008 Propagation of distributions using a Monte Carlo method → **MC simulation**

  ISO/IEC Guide 98-3/NP Suppl 2: Models with any number of output quantities → **MU propagation**

- **EURACHEM/CITAC Guide „Quanti-fying Uncertainty in Analytical Measurement“: 2012 (2000)** → **Kragten approach**

Principles: The three approaches in a nutshell

$$y = f(x_1,\ldots,x_n)$$

MU propagation

$$u^2(y) = \vec{J} \times \hat{V}(x_1,\ldots,x_n) \times \vec{J}^T$$

„Kragten approach“

$$u^2(y) = \sum_{i=1}^{n} [f(\ldots,x_i + u(x_i)/2,\ldots) - f(\ldots,x_i - u(x_i)/2,\ldots)]^2$$

pdf propagation

$$pdf(y) = \frac{\int\ldots\int pdf(x_1)\cdot\ldots\cdot pdf(x_n)\cdot dx_1\cdot\ldots\cdot dx_n}{\int p(y)\cdot dy}$$

MU propagation

$$\vec{f}(\vec{x},\vec{y}) = 0$$

$$\vec{y} = (y_1,\ldots,y_k) \qquad \vec{x} = (x_1,\ldots,x_n)$$

many output variables

$$\hat{V}(\vec{y}) = \hat{Q} \times \hat{V}(\vec{x}) \times \hat{Q}^T$$

$$Q = \hat{J}_y^{-1} \times \hat{J}_x \qquad \hat{J}_y = \{\frac{\partial f_k}{\partial y_m}\} \qquad \hat{J}_x = \{\frac{\partial f_k}{\partial x_i}\}$$

$$y = f(x_1,\ldots,x_n)$$

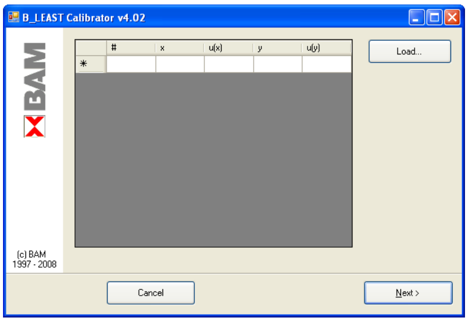
$$u^2(y) = \vec{J} \times \hat{V}(x_1,\ldots,x_n) \times \vec{J}^T$$

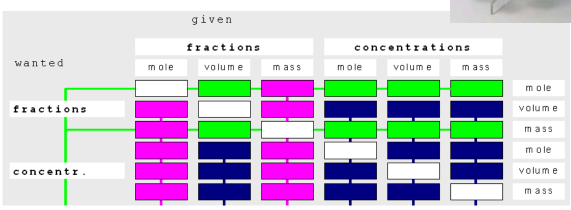
one output variable

$$\vec{J} = \{\frac{\partial f}{\partial x_i}\}$$

MU propagation applied

- piles of examples in „Accreditation and Quality Assurance“
- Generalised Least Squares Regression according to ISO 6143 software: B_Least, XGenLine
- Unit conversion of gas composition according to ISO 14912 software: CONVERT





BAM

The Kragten approach

$$\frac{\partial f}{\partial x_i} \approx \frac{f(\ldots, x_i + \delta, \ldots) - f(\ldots, x_i, \ldots)}{\delta} \quad and \quad \delta = u(x_i)$$

$$\frac{\partial f}{\partial x_i} \cdot u(x_i) \approx f(\ldots, x_i + u(x_i), \ldots) - f(\ldots, x_i, \ldots)$$

symmetric

$$u^2(y) = \sum_{i=1}^{n} [f(\ldots, x_i + u(x_i)/2, \ldots) - f(\ldots, x_i - u(x_i)/2, \ldots)]^2$$

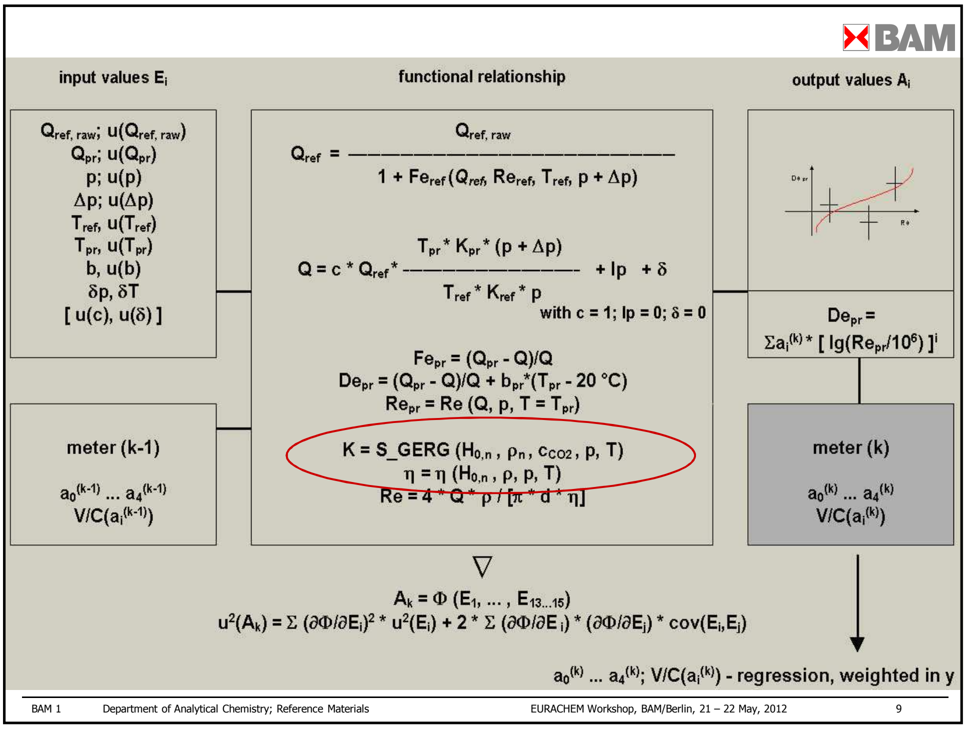
asymmetric

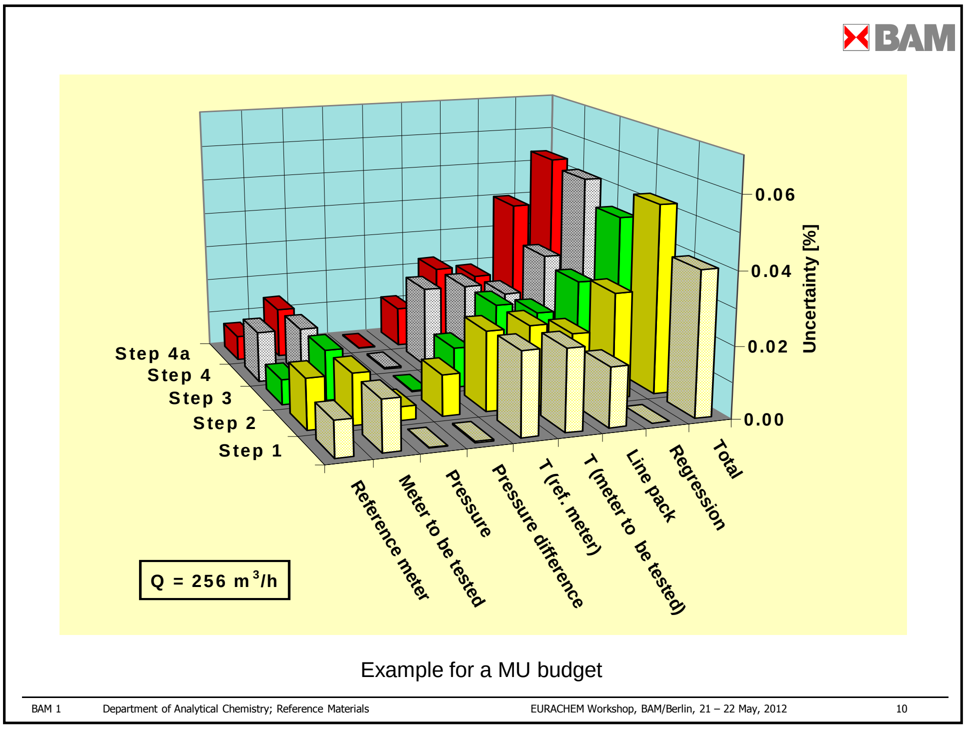
$$u^2(y) = \sum_{i=1}^{n} [f(\ldots, x_i + u(x_i), \ldots) - f(\ldots, x_i, \ldots)]^2$$

$$u^2(y) = \sum_{i=1}^{n} [f(\ldots, x_i, \ldots) - f(\ldots, x_i - u(x_i), \ldots)]^2$$

BAM

An application of the Kragten approach


BAM
input values E_i
functional relationship
output values A_i
Q_ref, raw; u(Q_ref, raw)
Q_pr; u(Q_pr)
p; u(p)
Δp; u(Δp)
T_ref, u(T_ref)
T_pr, u(T_pr)
b, u(b)
δp, δT
[u(c), u(δ)]
Q_ref = Q_ref, raw / (1 + Fe_ref (Q_ref, Re_ref, T_ref, p + Δp))
Q = c * Q_ref * (T_pr * K_pr * (p + Δp)) / (T_ref * K_ref * p) + Ip + δ
with c = 1; Ip = 0; δ = 0
Fe_pr = (Q_pr - Q)/Q
De_pr = (Q_pr - Q)/Q + b_pr*(T_pr - 20 °C)
Re_pr = Re (Q, p, T = T_pr)
K = S_GERG (H_0,n , ρ_n , c_CO2 , p, T)
η = η (H_0,n , ρ, p, T)
Re = 4 * Q * ρ / [π * d * η]
De_pr =
Σa_i^(k) * [lg(Re_pr/10^6)]^i
meter (k-1)
a_0^(k-1) ... a_4^(k-1)
V/C(a_i^(k-1))
meter (k)
a_0^(k) ... a_4^(k)
V/C(a_i^(k))
A_k = Φ (E_1, ... , E_13...15)
u²(A_k) = Σ (∂Φ/∂E_i)² * u²(E_i) + 2 * Σ (∂Φ/∂E_i) * (∂Φ/∂E_j) * cov(E_i,E_j)
a_0^(k) ... a_4^(k); V/C(a_i^(k)) - regression, weighted in y
BAM 1
Department of Analytical Chemistry; Reference Materials
EURACHEM Workshop, BAM/Berlin, 21 – 22 May, 2012
9


BAM
Step 4a
Step 4
Step 3
Step 2
Step 1
0.06
0.04
0.02
0.00
Uncertainty [%]
Reference meter
Meter to be tested
Pressure
Pressure difference
T (ref. meter)
T (meter to be tested)
Line pack
Regression
Total
Q = 256 m³/h
Example for a MU budget
BAM 1
Department of Analytical Chemistry; Reference Materials
EURACHEM Workshop, BAM/Berlin, 21 – 22 May, 2012
10

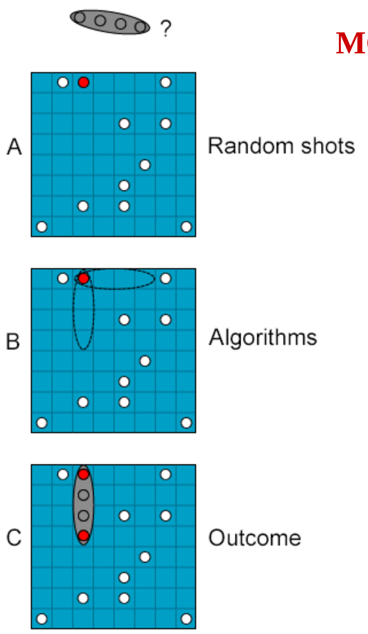
Monte Carlo simulation

The idea: Enrico Fermi (1930s) and Stanisław Ulam (1946)
Ulam later contacted John von Neumann to work on it.

The problem: In the 1940s, physicists at Los Alamos Scientific Laboratory were investigating radiation shielding and the distance that neutrons would likely travel through various materials. Despite having data such as the average distance a neutron would travel in a substance before it collided with an atomic nucleus or how much energy the neutron was likely to give off following a collision, the problem could not be solved with analytical calculations.

The name: von Neumann and Ulam suggested modeling the experiment on a computer. Being secret, this required a code. Von Neumann chose the name "Monte Carlo". The name is a reference to the Casino in Monaco where Ulam's uncle would borrow money to gamble.

MC principles

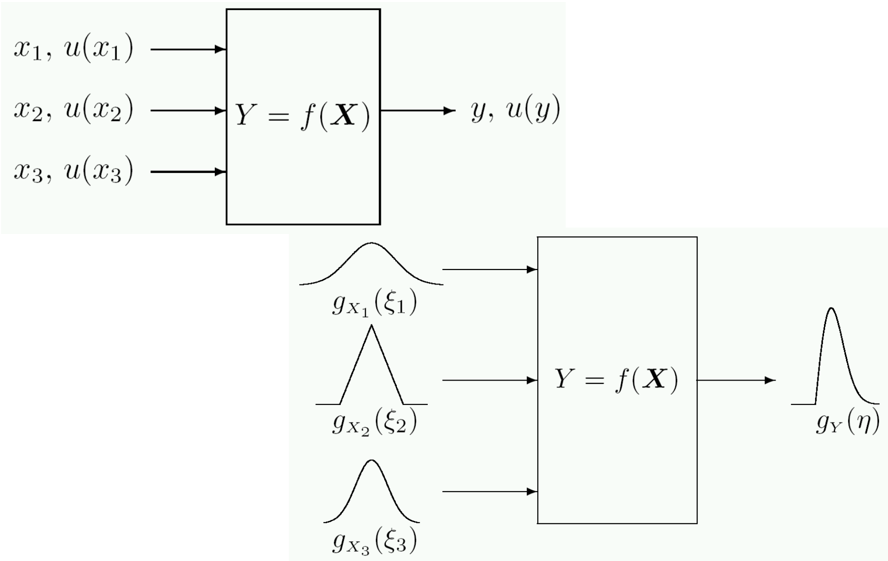


no single Monte Carlo method

general scheme:

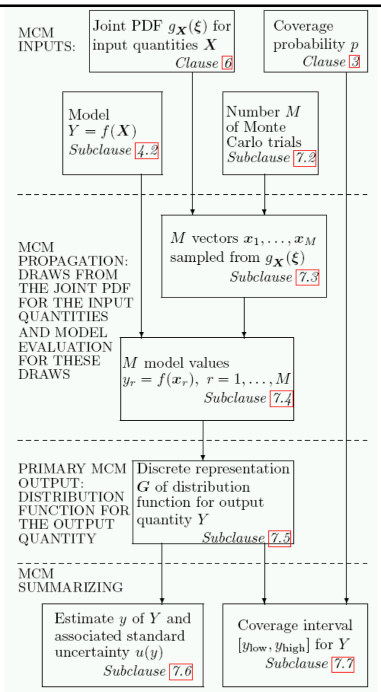
- Define a domain of possible inputs.
- Generate inputs randomly from the domain using a certain specified probability distribution.
- Perform a deterministic computation using the inputs.
- Aggregate the results of the individual computations into the final result.

Application to MU estimation (1)



BAM 1 Department of Analytical Chemistry; Reference Materials EURACHEM Workshop, BAM/Berlin, 21 – 22 May, 2012 13

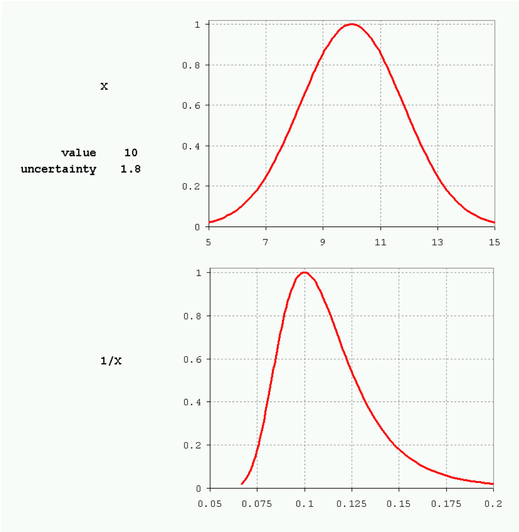
Application to MU estimation (2)



Input parameter	
n	Dimension of the multivariate Gaussian distribution
$\boldsymbol{\mu}$	$n \times 1$ vector of expectations
$\boldsymbol{V}$	Covariance matrix of order n
q	Number of multivariate Gaussian pseudo-random numbers to be generated
Output parameter	
$\boldsymbol{X}$	$n \times q$ matrix, the jth column of which is a draw from the multivariate Gaussian distribution
Computation	
	a) Form the Cholesky factor $\boldsymbol{R}$ of $\boldsymbol{V}$, i.e. the upper triangular matrix satisfying $\boldsymbol{V} = \boldsymbol{R}^{\mathrm{T}}\boldsymbol{R}$. (To generate q pseudo-random numbers, it is necessary to perform this matrix factorization only once.) b) Generate an $n \times q$ array $\boldsymbol{Z}$ of standard Gaussian variates c) Form $$\boldsymbol{X} = \boldsymbol{\mu}\boldsymbol{1}^{\mathrm{T}} + \boldsymbol{R}^{\mathrm{T}}\boldsymbol{Z},$$ where $\boldsymbol{1}$ denotes a column vector of q ones

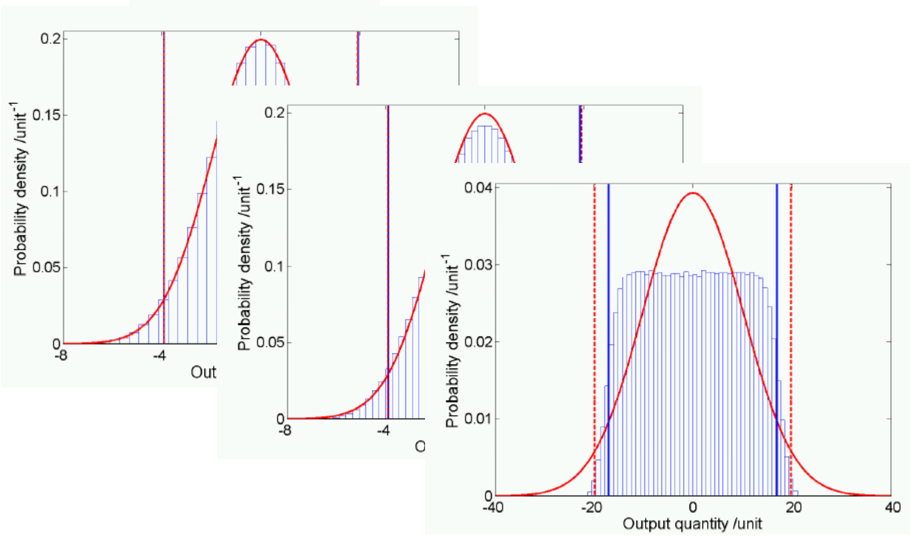
BAM 1 Department of Analytical Chemistry; Reference Materials EURACHEM Workshop, BAM/Berlin, 21 – 22 May, 2012 14

Problem 1: Large uncertainties



Problem 2: Distributions deviating from normal

$$Y = X_1 + X_2 + X_3 + X_4,$$



Benefits and limitations

	GUM approach	MC simulation
function f(x)	linearisation (Taylor series development)	any, also non-linear, as is
input uncertainties	small, best if < 0.03	any, even very large
output uncertainty	always symmetric	may be (strongly) asymmetric and kurtic
handling of output	guidelines exist	undefined
coverage interval	standard (expanded by t or k)	may be (quite) different from standard
efforts	moderate (after 15 years of teaching, even routine labs should understand the concept)	high to very high (programming required, solutions are tailored)

Beyond MU: Performance of a regression method

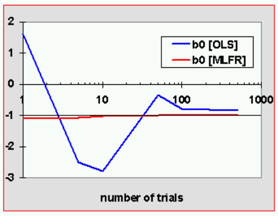


Fig. 1a: Analysis function intercept in dependence on the number of trials

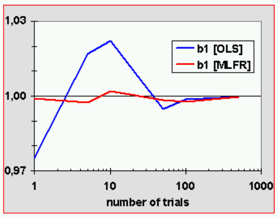


Fig. 1b: Analysis function slope in dependence on the number of trials

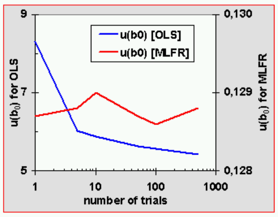


Fig. 1c: Intercept uncertainty in dependence on the number of trials

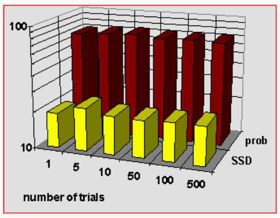


Fig. 1d: True-prediction probability (scale in %) and residual SSD

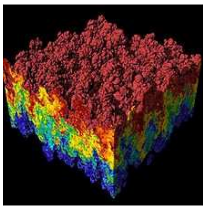
Bremser, W., and Hässelbarth, W.: Uncertainty-based calibration for wide measuring ranges

1st Int. Forum Intelligent Analytical Solutions, Jülich, 24-26 September 1998

BAM

Conclusions

- Propagation of uncertainty (standard GUM) works well with small uncertainties or linear model functions.
- Numerical methods can handle larger uncertainties, non-linear and/or non-analytical model functions.
- Monte Carlo simulation is a mighty tool in computational mathematics with wide-spread applications in physics, chemistry, telecommunications. Applied to measurement uncertainty, it extends the standard GUM approach from uncertainty propagation to probability-distribution-function (pdf) propagation. It can handle non-linear and even problems with singularities (constraints) as well as large uncertainties.
- The outcome may be a skewed and/or kurtic pdf requiring the statement of asymmetric uncertainties, amended coverage intervals, and averages deviating from any straightforward estimates. Computation may require considerable efforts. MU estimation using MC is not recommended for routine applications.



Thank you for your attention!

BAM 1 Department of Analytical Chemistry; Reference Materials EURACHEM Workshop, BAM/Berlin, 21 – 22 May, 2012 19