TOP-DOWN
Uncertainty estimation

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Two ways for determining the uncertainty

Top down

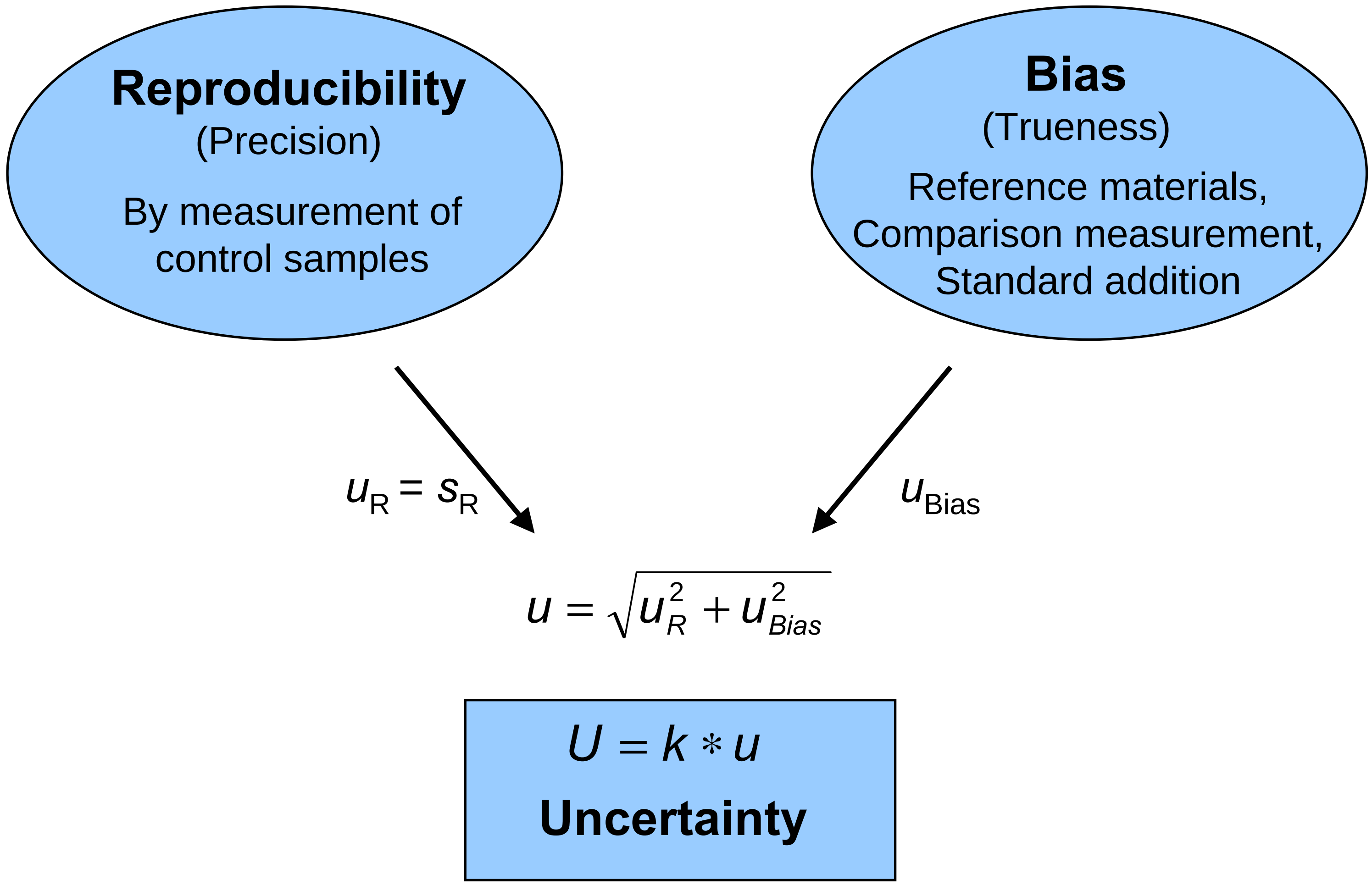
Phenomenological approach
basing on validation and QC data
assuming that they
- cover all influence factors and
- that they are representative
  for all measurements with
  this method

According to GUM
starting from the
model equation and
considering all individual
uncertainty contributions

Bottom up

Top-down appraoch

according to „Nordtest“:



Top Down example

Example : Uncertainty estimation using data (***s*** , **Δ)** from a validation of the measurement procedure by means of a CRM

Precondition: The composition of the samples should be similar to that of the CRM in order to be able to apply the validation data for future measurements

Parameter: ***s*** precision, **Δ** trueness

Validation by means of a CRM

Measurement result for the CRM:

Mean value $\bar{x}$ from n single measurement results x_k under repeatebility conditions, as those expected for further measurements.

Certified reference value: x_{ref}

Systematic deviation: $\Delta = \bar{x} - x_{\mathrm{ref}}$

Standard deviation: $s = \sqrt{\frac{1}{n-1}\sum_{k=1}^{n}(x_k - \bar{x})^2}$

Uncertainty and Significance Test

Uncertainty of Δ:

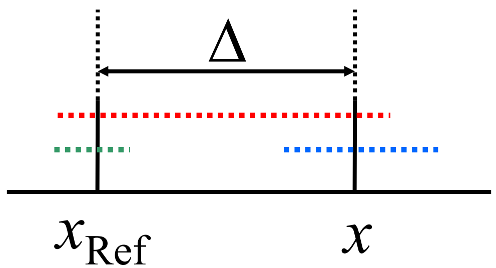
$$2u(\Delta) = 2\sqrt{u^2(\bar{x}) + u^2(x_{ref})} = 2\sqrt{\frac{s^2}{n} + u^2(x_{ref})}$$

Measurements of the CRM ($\frac{s^2}{n}$)   Certified RM ($u^2(x_{ref})$)

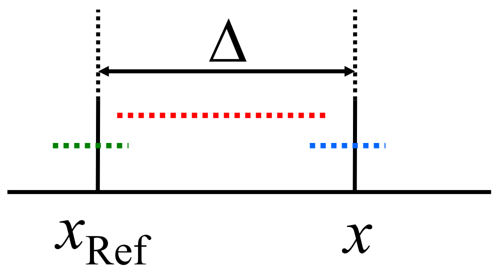
Test criteria for the relevance of the deviation

$$2u(\Delta) \geq \quad |\Delta| \quad > 2u(\Delta)$$

Not significant



Significant



Correction for Δ

a) Δ is significant → correction of *y*

$$y_{\text{korr}} = y - \Delta$$

$$u(y_{\text{korr}}) = \sqrt{s^2 + u^2(\Delta)} = \sqrt{s^2 + \frac{s^2}{n} + u^2(x_{\text{ref}})}$$

- Repeat measurements of the sample → s^2
- Repeat measurements of CRM → $\frac{s^2}{n}$
- CRM → $u^2(x_{\text{ref}})$

Integration of Δ in the uncertainty

b) Δ significant but no correction of *y*:

Instead of that consideration of the deviation in the uncertainty.

$$u(y) = \sqrt{u^2(y_{\text{korr}}) + \Delta^2} = \sqrt{s^2 + u^2(\Delta) + \Delta^2}$$

$$= \sqrt{s^2 + \frac{s^2}{n} + u^2(x_{\text{ref}}) + \Delta^2}$$

Repeat measurements of the sample

Repeat measurements of CRM

CRM

Bias

Integration of Δ in the uncertainty

c) Δ is not significant ⟶ no correction of *y*

$$u(y_{\text{nichtkorr}}) = \sqrt{u^2(y_{\text{korr}}) + \Delta^2} = \sqrt{s^2 + u^2(\Delta) + \Delta^2}$$

Same expression as for b)

$$= \sqrt{s^2 + \frac{s^2}{n} + u^2(x_{\text{ref}}) + \Delta^2}$$

- Repeat measurements of the sample
- Repeat measurements of CRM
- CRM
- Bias

Proportional deviation

Δ is proportional to the magnitude of the quantity

Recovery: $$R = \frac{\bar{x}}{x_{ref}}$$ and $$R - 1 = \frac{\Delta}{x_{ref}}$$

Multiplicative correction useful: $$y_{korr} = y * \frac{1}{R}$$

Is Δ significant then ***R*** is also significant

Correction for *R*

a) *y* is corrected for *R*:

$$u_{\text{rel}}(y_{\text{korr}}) = \sqrt{s_{\text{rel}}^2 + u_{\text{rel}}^2(R)} \qquad \text{and} \qquad s_{\text{rel}} = \frac{s}{y}$$

$$= \sqrt{s_{\text{rel}}^2 + \frac{s_{\text{rel}}^2}{n} + u_{\text{rel}}^2(x_{\text{ref}})}$$

Repeat measurements of the sample

Repeat measurements of CRM

CRM

Integration of *R* in the uncertainty

b) *y* needs not to be corrected

because ***R*** don‘t differ enough from 1

$$u_{rel}(y_{nichtkorr}) = \sqrt{s_{rel}^2 + u_{rel}^2(R) + (R-1)^2}$$

$$= \sqrt{s_{rel}^2 + \frac{s_{rel}^2}{n} + u_{rel}^2(x_{ref}) + (R-1)^2}$$

Repeat measurements of the sample

Repeat measurements of CRM

CRM

Bias

Uncertainty estimations by means of other data

Comparison measurements:

$$2\,u(\Delta) = 2\sqrt{s^2 + \frac{\sum \Delta_R^2}{n_R} + \frac{\sum 1{,}25^2 \cdot \frac{s_{R,i}^2}{n_{T,i}}}{n_R}}$$

Mean of the deviations

Mean standard uncertaity of the reference value

Standard addition:

$$2\,u(\Delta) = 2\sqrt{s^2 + \frac{\sum \Delta_R^2}{n_R} + u_{Vol}^2 + u_{S\tan dard}^2}$$

Volume measurement

Added standard solution

Hg measurement (natural water sample)

PTB

in ng/l

x_1 = 546
x_2 = 546
x_3 = 588
x_4 = <u>553</u>
x_m = 558

$s\ (x_m)$ = 20
$u\ (x_m)$ = 10
$u\ (x_{ref})$ = 7
Δ = -24

$$2u(\Delta) = 2\sqrt{\frac{s^2}{n} + u^2(x_{ref})}$$

$$2u(\Delta) = 2 * \sqrt{10^2 + 7^2} = 24$$

$$u(y_{korr}) = \sqrt{s^2 + u^2(\Delta)} = \sqrt{s^2 + \frac{s^2}{n} + u^2(x_{ref})}$$

$u\ (y_{korr})$ = $\sqrt{20^2 + 10^2 + 7^2}$ = 24

$u_{rel}(y_{korr})$ = 4,1%

$U(Y_{korr})$ = $u\ (y_{korr})$ *2 = 47

y_{korr} = $x_m - \Delta$

x_{ref} = 582 ng/l

Y_{korr} = <u>(582 ± 47) ng/l</u>

Hg measurement (natural water sample)

$$u(y_{korr}) = \sqrt{s^2 + u^2(\Delta)} = \sqrt{s^2 + \frac{s^2}{n} + u^2(x_{ref})}$$

Y_{korr} = (582 ± 47) ng/l

x_{ref} = 0,582 ng/l

$$u(y) = \sqrt{u^2(y_{korr}) + \Delta^2} = \sqrt{s^2 + u^2(\Delta) + \Delta^2}$$

$$u(y) = \sqrt{20^2 + 10^2 + 7^2 + 24^2} = 34$$

$u_{rel}(y)$ = 5,9%

Y =(558 ± 67) ng/l

Thanks for your attention

Basic equation for the statistical model

According to ISO/TS 21748:

$$\boldsymbol{y = \mu + \delta + B + \Sigma c_i x_i + e}$$

$$\boldsymbol{u^2(y) = u^2(\delta) + s_L^2 + \Sigma c_i^2 u^2(x_i) + s_r^2}$$

y	*observed result*
μ	*expectation value of the result*
δ	*intrinsic bias*
B	*laboratory bias*
x_i	*deviation from the nominal value*
c_i	*sensitivity coefficient*
e	*random residual error*

s_L^2	variance of B *(certified)*
s_r^2	variance of e
$u^2(\delta)$	variance due to the measurement of RM
$u^2(x_i)$	