Scoring systems for quantitative schemes – what are the different principles ?

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ISO/IEC 17043
4.7.2 Evaluation of performance

- **4.7.2.1 The proficiency provider shall use valid methods of evaluation which meet the purpose of the proficiency testing scheme. The methods shall be documented and include a description of the basis for the evaluation.**

ISO/IEC 17043 - Annex B.3 – Calculation of performance statistics

- Transformation of PT results into a performance statistic for interpretation and comparison purposes
- The purpose is to measure the deviation from the assigned value in a manner that allows comparison with performance criteria.

ISO/IEC 17043 - Annex B.2 Assigned value

1. Formulation
2. Certified reference value
3. Reference value
4. Consensus value from expert laboratories
5. Consensus value from participant‘s data

ISO/IEC 17043 - Annex B.3 – Standard deviation for proficieny assessment

1. Prescribed value
2. By perception
3. Statistical model
4. From results of precision experiments
5. From participant results

SDPA – Prescribed value

- SDPA may be set at a value required for a specific task of data interpretation
- Determined by expert judgement or regular mandate
- From „outside of the PT system“
- E.g.: Directive (2009/90/EC) from the european comission to the WFD:
  - Analytical method can have a max. uncertainty of 25 % at the EQS

SDPA – by perception

- Choice according to a „fitness-for-purpose“-wish for the laboratory
- Estimate from previous rounds of proficiency testing or expectations based on experience
- From „inside of the PT system“

SDPA – from a statistical model

- Value of the SDPA is derived from a general model for the reproducibility of the measurement method (e.g. Horwitz curve)
  - Reproducibility SD is a function from the concentration (mass fraction)

SDPA – from the results of a precision experiment

- When one standardised method is used in the PT
- Requirement:
  - Information of the repeatability and reproducibility must be available

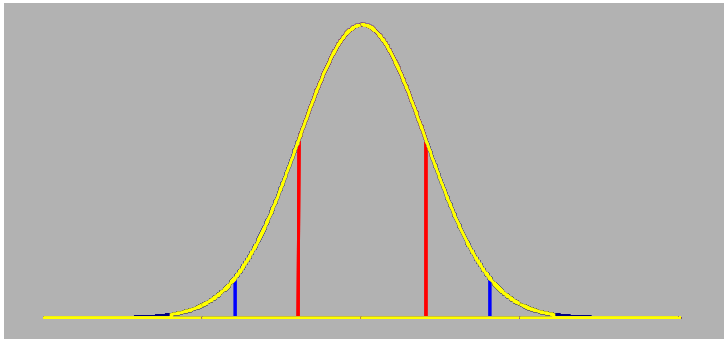
Calculation of the SDPA using this information

SDPA – from data obtained in a round of a proficiency testing scheme

- Calculated with robust statistic from the results of the participants in PT
- ISO/TS 20612:
  - Q-method
  - Application of a variance function
- ISO 13528
  - Algorithm A

Performance scoring
Normal distribution – important properties

- The curve is symmetrical about the population mean μ
- The greater the value of σ the greater the spread of the curve
- Approximately 68% (68,27%) of the data lie within μ±1σ
- Approximately 95 % (95,45%) of the data lie within μ±2σ
- Approximately 99,7 % (99,73%) of the data lie within μ±3σ



$$y = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{(x-\mu)^2}{2\sigma^2}}$$

Estimate of laboratory bias D – percent difference $D_{\%}$

- Estimate of laboratory bias: $D = (x - X)$
- x: participant‘s result
- X: assigned value
- Percent difference $D_{\%}$: $D_{\%} = \frac{(x - X)}{X} * 100$

- Independent of the magnitude of the assigned value

Interpretation of differences

- Warning signal if: $2\,\hat{\sigma} < D < -2\,\hat{\sigma}$
- Action signal if: $3\,\hat{\sigma} \leq D \leq -3\,\hat{\sigma}$

- Advantage:
  - Easy to understand
- Disadvantage:
  - not standardised to allow simple scanning for action signals

Calculation of performance statistics – z-score

$$z = \frac{(x - X)}{\hat{\sigma}}$$

x result of the participant

X assigned value

$\hat{\sigma}$ SDPA

Adoption: data set is normal distributed

Interpretation of z-scores

z-score:

$|z| \leq 2{,}0 \Rightarrow$ satisfactory

$2{,}0 < |z| < 3{,}0 \Rightarrow$ questionnable (warning signal)

$|z| \geq 3{,}0 \Rightarrow$ unsatisfactory (action signal)

- Advantage:
  - Standardised score
  - Most commonly used
- Disadvantage:
  - Performance assessment depends on the choice of SDPA

z‘-score

$$z' = \frac{(x - X)}{\sqrt{\hat{\sigma}^2 + u_x{}^2}}$$

u_x standard uncertainty of the assigned value

- Application of z-scores, if:

$$u_x \leq 0{,}3\hat{\sigma}$$

- Otherwise the uncertainty of the assigned value is not negligible
- Then the possibility is given that z-values deliver a warning or action signal, but not the z‘-values

zeta-score (ζ-score)

$$\zeta = \frac{x - X}{\sqrt{u_x^{\,2} + u_X^{\,2}}}$$

- u_x estimate of the standard uncertainty from the result of the laboratory
- u_X standard uncertainty from the assigned value

ζ-score:

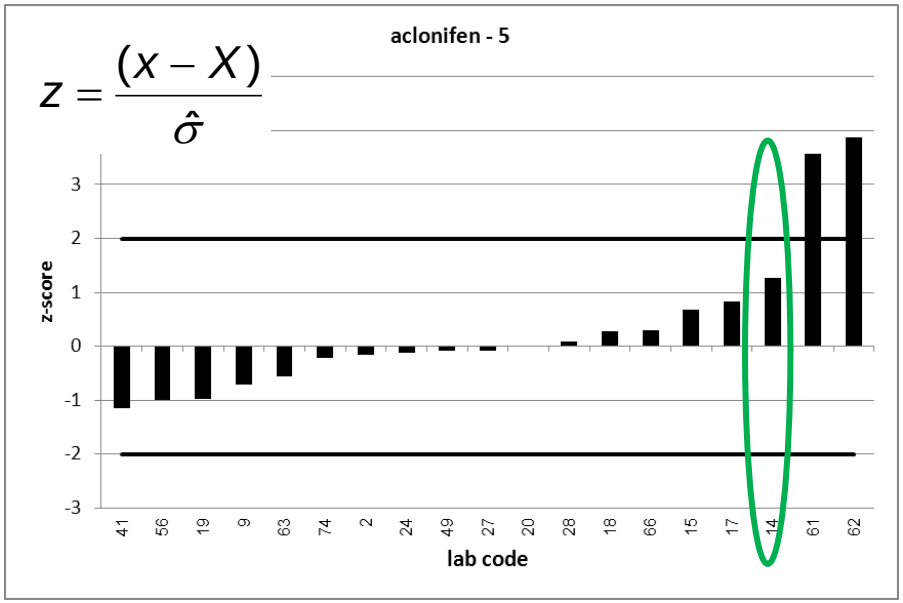
$|\zeta| \leq 2{,}0 \Rightarrow$ satisfactory

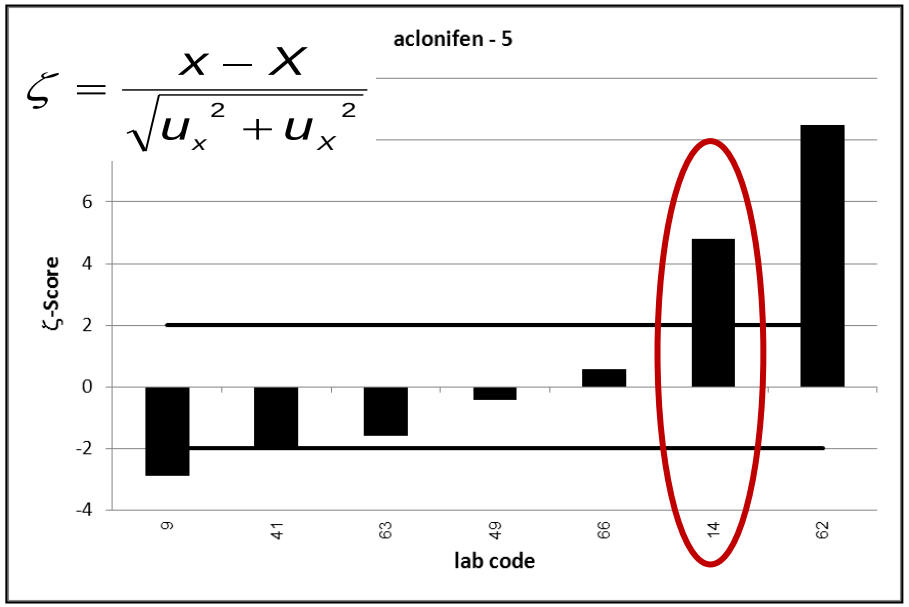
$2{,}0 < |\zeta| < 3{,}0 \Rightarrow$ questionnable (warning signal)

$|\zeta| \geq 3{,}0 \Rightarrow$ unsatisfactory (action signal)

Interpretation of ζ-scores

- ζ-scores can be used together with z-scores to check the plausiblity of the estimation of measurement uncertainty





E_n-number

$$E_n = \frac{x - X}{\sqrt{U_{lab}^{\ 2} + U_{ref}^{\ 2}}}$$

- *X* assigned value derived from a reference laboratory
- U_{ref} *expanded uncertainty from X*
- U_{lab} expanded uncertainty from the result x of a laboratory
- Applied in key comparisons of metrology institutes

E_n-number:

$|E_n| \leq 1{,}0 \Rightarrow$ satisfactory

$|E_n| > 1{,}0 \Rightarrow$ unsatisfactory

Laboratory assessment

© Koch, M.: Interlaboratory tests In: Wenclawiak, Koch, Hadjicostas (eds): Quality Assurance in Analytical Chemistry – Training and Teaching (2nd edition), Springer Verlag, Berlin Heidelberg 2010

- By combination of single value assessment
- Involves danger of missinterpretation
  - A laboratory can measure one parameter permanently wrong, but nevertheless is positive assessed

Combined Assessment According to IUPAC – RSZ

- RSZ (rescaled sum of z-scores)
  - RSZ = $\Sigma z/\sqrt{m}$ with m = number of scores
  - Same scale as z-score
  - Negative assessment, if all values are within the tolerance but a little biased in the same direction
  - Errors with opposite sign cancel each other out

Combined Assessment According to IUPAC – SSZ

- SSZ (sum of squared z-scores)
  - Does not consider the sign of z-scores

Control charts