Multivariate and correlated acceptance limits for conformity assessment

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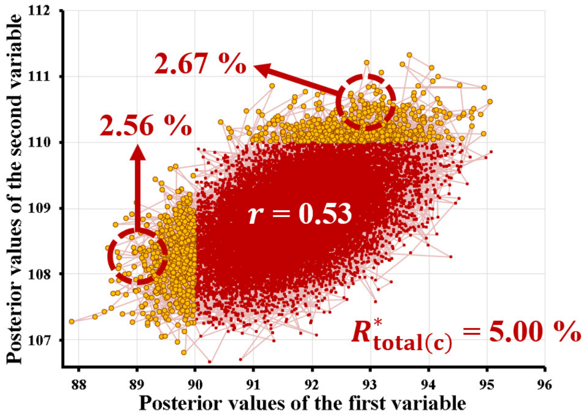

**Berlin,
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Outline

1. Frequentist and Bayesian uncertainty evaluations
2. Multivariate Bayesian conformity assessment
3. MS-Excel tool for defining acceptance limits
4. Application examples
5. Conclusion

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1. Frequentist and Bayesian uncertainty evaluations

The measurement uncertainty evaluation can be:

- **Frequentist (classical)**
- **Bayesian**

Bayesian evaluations use available prior information on the studied measurand (…) to improve the measurement result.

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1. Frequentist and Bayesian uncertainty evaluations

Bayesian reasoning example:
Simple qualitative analysis example:

Pregnancy testing from fast kits:
True positive results rate, *TP*: 98.5 %
False positive results rate, *FP*: 0.8 %

A frequentist would say that tested woman has a 50 % probability of being pregnant, therefore, the probability of a positive result being correct, *P* is:

$$P = \frac{98.5\ \%}{98.5\ \% + 0.8\ \%} = 99.2\ \%$$

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(…) however, a Bayesian would ask woman's age and take pregnancy prevalence into account. For a 28 years old woman, since 16.2 % of woman are pregnant:

$$P = \frac{98.5\ \% \cdot 16.2\ \%}{98.5\ \% \cdot 16.2\ \% + (100\% - 16.2\ \%)0.8\ \%} = 96.0\ \%$$

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For a 44 years old woman, since 1.9 % are pregnant:

$$P = \frac{98.5\ \% \cdot 1.9\ \%}{98.5\ \% \cdot 1.9\ \% + (100\% - 1.9\ \%)0.8\ \%} = 70.4\ \%$$

Pregnancy prevalence depends on the country. Since considered prevalence has a major impact on result, it must be carefully selected.

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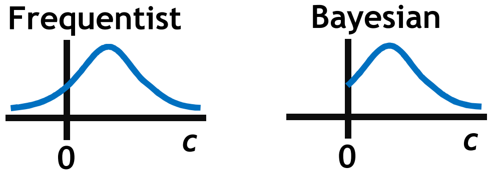
1. Frequentist and Bayesian uncertainty evaluations

Bayesian inference is applicable to continuous variables problems, such as the measurement of a concentration and the assessment of the compliance of a product given a concentration limit.

In measurements in chemistry, the prior information can be:

- Concentration cannot be negative;
- Mass fraction is ≥ 0 and ≤ 1;



- In some cases, records from results of the analysis of samples equivalent to the analysed one can be considered…; prior information must be adequate.

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2. Multivariate Bayesian conformity assessment

Conformity assessment can be based on:

» Risk calculation and comparison with a maximum risk (e.g. maximum consumer's risk of 5 %)
Example: Consumer's risk is 1.3 %. Since the maximum consumer's risk is 5 %, product is conforming.

» Acceptance limit calculation (concentration associated with the maximum risk) and comparison of the measured concentration with the acceptance limit.
Examples: Measured concentration is 3.20 mg/L and the maximum acceptance limit is 3.09 mg/L; therefore, product does not conform.

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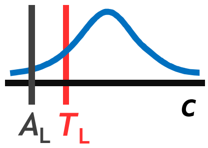
2. Multivariate Bayesian conformity assessment

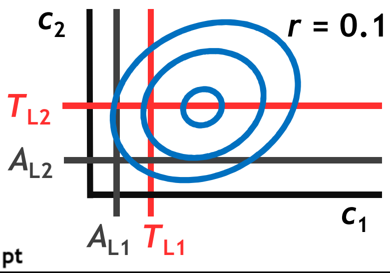
Conformity assessment can be univariate:

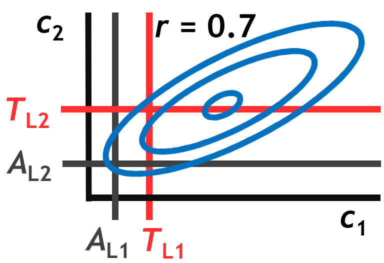
Acceptance limit, A_L

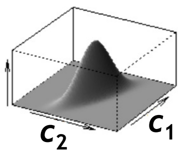
Tolerance Limit, T_L



Conformity assessment can be multivariate (for instance, bivariate):







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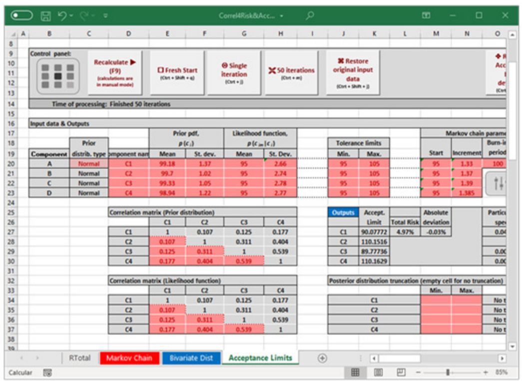
3. MS-Excel tool for defining acceptance limits

A MS-Excel spreadsheet was developed to defined multivariate acceptance limits for Bayesian assessments based on a tool developed by Kuselman et al. [1].

Input data:
- Prior data;
- Tolerance limit(s);
- Measurement uncertainty;
- Type of reference risk (consumer's or producer's);
- Maximum total risk.



1 - I. Kuselman, F. Pennecchi, R. B. Silva, D. B. Hibbert, IUPAC project 2016-007-1-500: Risk of conformity assessment of a multicomponent material or object in relation to measurement uncertainty of its test result, 2016 - 2018.

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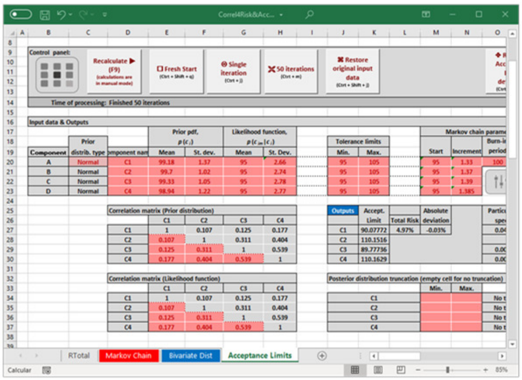
Determination of acceptance limits by iteration of risks determinations by:

Markov chain Monte Carlo Method.



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4. Application examples

Examples of the determination of acceptance limits for a 5 % particular or total specific consumer's risk.

Case	Prior	Likelihood	$[T_{Li}, T_{Ui}]$	A_L	A_U
1	Normal μ_1 = 99.18; σ_1 = 1.37	Normal $u_1 = 0.028c_{1m}$	[95, 105]	A_{L1} = 89.935	A_{U1} = 126.56
2	Uniform μ_1 = U(0; -)	Normal $u_1 = 0.028c_{1m}$	[95, 105]	$R^*_{c1(c)}$ (%) > 7.54 (value for c_{1m} = 100)	
A_L – Lower acceptance limit; A_U – Upper acceptance limit; Neg. Correl. - Negligible correlation.					

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3	Normal μ_1 = 99.18; σ_1 = 1.37; μ_2 = 99.70; σ_2 = 1.02 μ_3 = 99.33; σ_3 = 1.05; μ_4 = 98.94; σ_3 = 1.22 Correlation coefficients: r_{12} = 0.107; r_{13} = 0.125; r_{14} = 0.177; r_{13} = 0.311; r_{24} = 0.404; r_{34} = 0.539	Normal $u_1 = 0.028c_{1m}$ u_2 = 2.74 u_3 = 2.78 u_4 = 2.77 Correlation coefficients (see Prior)	[95, 105]	A_{L1} = 90.281 A_{L2} = 91.44 A_{L3} = 90.558 A_{L4} = 90.449	A_{U1} = 124.15 A_{U2} = 120.192 A_{U3} = 121.357 A_{U4} = 121.35
4	Case 3 but Neg. Correl.	Case 3 but Neg. Correl.	[95, 105]	A_{L1} = 92.463 A_{L2} = 91.82 A_{L3} = 91.322 A_{L4} = 91.223	A_{U1} = 123.42 A_{U2} = 119.639 A_{U3} = 120.791 A_{U4} = 120.709
5	Uniform μ_1 = U(0; -); μ_2 = U(0; -); μ_3 = U(0; -); μ_4 = U(0; -); Neg. Correl.	Case 3	[95, 105]	$R^*_{\mathrm{total(c)}}$ (%) > 23.32 (value for c_{1m}, c_{2m}, c_{3m} and c_{4m} = 100)	
6	Case 5	Case 3 but Neg. Correl.	[95, 105]	$R^*_{\mathrm{total(c)}}$ (%) > 24.89 (value for c_{1m}, c_{2m}, c_{3m} and c_{4m} = 100)	

A_L – Lower acceptance limit; A_U – Upper acceptance limit; Neg. Correl. - Negligible correlation.

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5. Conclusion

● **The developed tool makes complex conformity assessments easy!**

● **The easy comparison of various conformity assessments (e.g. based on informative or non-informative priors) allow understanding the conformity problem.**

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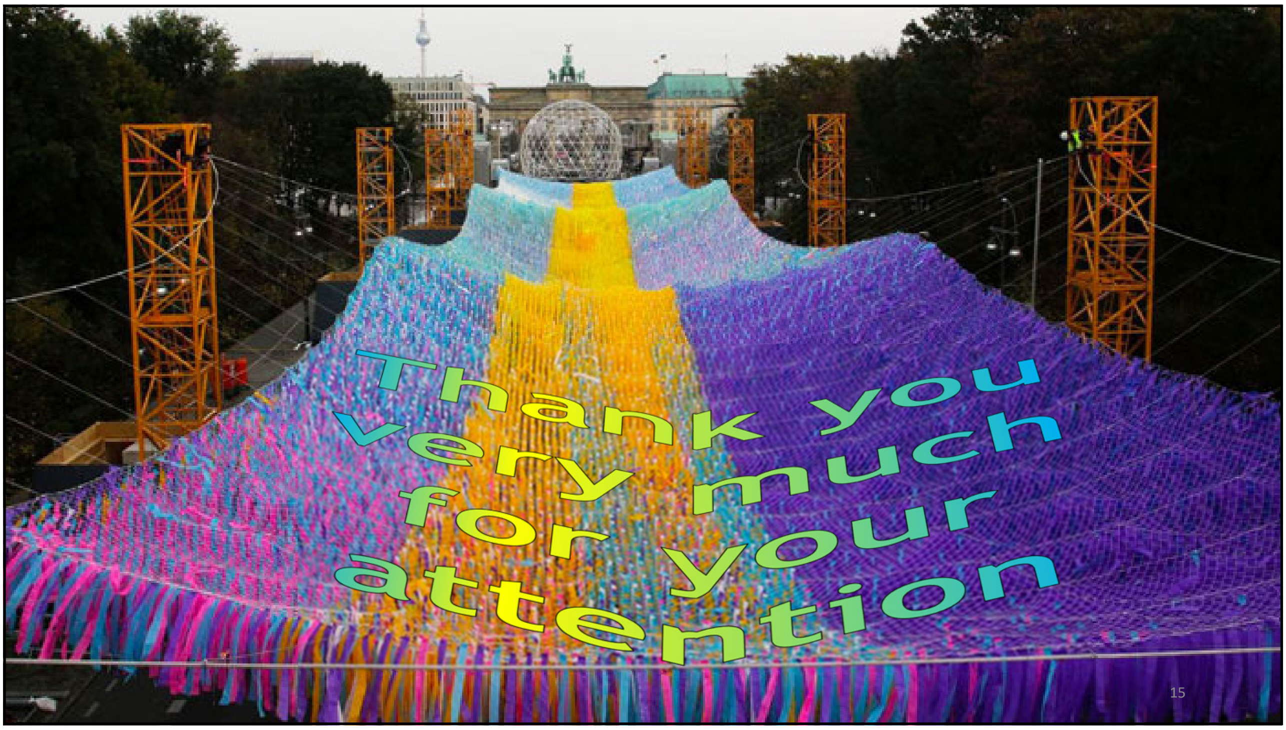
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