# Advanced methods for assessment of chemical compositions of multicomponent substances or materials and their categorical property values

# Advanced methods for assessment of chemical compositions of multicomponent substances or materials and their categorical property values

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## 1. Conformity Assessment of a Chemical Composition

A Bayesian methodology for the evaluation of risks of false decisions on conformity of a multicomponent substance, material or object, due to measurement uncertainty was developed and published as the IUPAC/CITAC Guide [Kuselman et al.(2021a)]. In continuation of this development, another IUPAC/CITAC Guide, taking into account a mass balance constraint of the object composition [Kuselman et. al.(2019)], is now under preparation for publication.

The mass balance constraint means, according to the law of conservation of mass, that the sum of the actual ('true') values of the component contents under conformity assessment is equal to 100 % (or 1 when expressed as fractions). At the same time, the sum of measured contents can differ from 100 % (or 1) because of measurement uncertainty. As a consequence, the actual component contents are intrinsically correlated. This correlation influences the evaluation of risks of false decisions in addition to effects of possible contributions of metrological, native or technological correlations of the data. The Guide will be helpful for a range of applications in analytical chemistry and metrology.

Different scenarios of risks of false decisions due to measurement uncertainty at the mass balance constraint are considered in the following examples of conformity assessment of chemical compositions of:

- a platinum-rhodium alloy produced by a manufacturer in a two-year period [Pennecchi et. al. (2020)];
- a batch of potassium iodate as a candidate reference material of given purity [Pennecchi et. al.(2021a)];
- sausage "Braunschweigskaya" from two manufacturers produced over three years [Pennecchi et. al.(2021b)];
- synthetic air prepared by NMIs as 'zero or balance gas' in calibration mixtures for Key Comparisons, and also by an industrial manufacturer for medicinal purposes [Pennecchi et. al.(2022)].

## 2. Assessment of Categorical Property Values

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Application of a newly-developed decomposition of total variation in two-way categorical analysis of variation of nominal values (CATANOVA) [Gadrich et al.(2020)], and two-way analysis of variation of ordinal values (ORDANOVA) [Gadrich & Marmor(2021)] for interlaboratory or similar comparisons of examination/test results, has been targeted in the next IUPAC project [Kuselman et al.(2021b)]. Two-way CATANOVA has been applied for interlaboratory examination of weld imperfections [Gadrich et al.(2020)]. A case study of expert responses of 45 ecological laboratories to intensity of odor and taste of drinking water was an example of the application of ORDANOVA [Gadrich et al.(2022a)]. Another example was a study of sensory responses of experts to the quality properties of samples of market-purchased sausage "Moscowskaya" manufactured by 16 producers. Dependence of the probabilities of classification of five quality properties to one of the categories as a function of the chemical composition of the sausage was assessed using multinomial ordered logistic regression [Gadrich et al.(2022b)].

## References


1 Gadrich T., Kuselman, I., Andrić, I.: Macroscopic examination of welds - Interlaboratory comparison of nominal data. SN Appl. Sci. (2020) 10.1007/s42452-020-03907-4

2 Gadrich T. and Marmor Y.N.: Two-way ORDANOVA - analyzing ordinal variation in a cross-balanced design. J. Stat. Plan. Inference (2021) doi: 10.1016/j.jspi.2021.04.005

3 Gadrich, T., Kuselman, I., Pennecchi F. R., Semenova, A.A., Chew, P.S., Naidenko, V.N.: Interlaboratory comparison of the intensity of drinking water odor and taste by two-way ordinal analysis of variation. J. Water Health (2022a) doi: 10.2166/wh.2022.060

4 Gadrich, T., Kuselman, I., Pennecchi F.R., Hibbert, D.B., Semenova, A.A., Chew, P.S.: Ordinal analysis of sensory responses in combination with multinomial ordered logistic regression vs. chemical composition. J. Food Qual. (2022b) doi: 10.1155/2022/4181460

5 Kuselman, I., Pennecchi, F.R., Hibbert, D.B., Di Rocco, A., Botha, A.: Influence of mass balance constraint on uncertainty of test results of a substance or material and risks in its conformity assessment. IUPAC Project (2019) https://iupac.org/project/2019-012-1-500

6 Kuselman, I., Pennecchi, F.R., da Silva, R.J.N.B., Hibbert, D.B.: IUPAC/CITAC Guide: Evaluation of risks of false decisions in conformity assessment of a multicomponent material or object (IUPAC Technical Report). Pure Appl. Chem. (2021a) doi: 10.1515/pac-2019-0906

7 Kuselman, I., Gadrich, T., Pennecchi, F.R., Hibbert, D.B., Semenova, A.A., Chew, P.S.: Harmonization of approaches to comparison of qualitative and related property values of a substance or material. IUPAC Project (2021b) https://iupac.org/project/2021-017-2-500/

8 Pennecchi, F.R., Di Rocco, A., Kuselman, I., Hibbert, D.B., Sega, M.: Correlation of test results and influence of a mass balance constraint on risks in conformity assessment of a substance or material. Measurement (2020) doi: 10.1016/j.measurement.2020.107947

9 Pennecchi, F.R., Kuselman, I., Di Rocco, A., Hibbert, D.B., Sobina, A., Sobina, E.: Specific risks of false decisions in conformity assessment of a substance or material with a mass balance constraint. Measurement (2021a) doi: 10.1016/j.measurement.2020.108662

10 Pennecchi, F.R., Kuselman, I., Di Rocco, A., Hibbert, D.B., Semenova, A.A.: Risks in a sausage conformity assessment due to measurement uncertainty, correlation and mass balance constraint. Food Control (2021b) doi: 10.1016/j.foodcont.2021.107949

11 Pennecchi, F.R., Kuselman, I., Hibbert, D.B., Sega, M., Rolle, F., Altshul V.: Fit-for-purpose risks in conformity assessment of a substance or material – A case study of synthetic air. Measurement (2022) doi: 10.1016/j.measurement.2021.110542