Extension of the JCGM 106:2012 - Conformity assessment of multicomponent items and finite statistical

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Editors: Rosaria Lombardo, Ida Camminatiello and Violetta Simonacci

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Extension of the JCGM 106:2012 - Conformity assessment of multicomponent items and finite statistical samples

Estensione del JCGM 106:2012 - Valutazione di conformità di oggetti multicomponente e campioni di numerosità finita

Francesca Pennecchi and Ilya Kuselman

Abstract The JCGM 106:2012 document provides guidelines on how to perform conformity assessment of a (scalar) property of interest of a single item (a product, material, object, etc.). In particular, based on a Bayesian approach, it indicates how to model and calculate specific and global risks of the consumer and the producer. In the present work, the JCGM 106 approach is generalized to items that are multicomponent materials (each component having its own property that should undergo conformity assessment with respect to its own requirements), and to a set of *N* items drawn from a common population (the probability of having a certain number of conforming items within this sample needs to be calculated).

Abstract *Il documento JCGM 106:2012 fornisce indicazioni su come effettuare la valutazione di conformità di una grandezza (scalare) di interesse, relativa ad una singola entità (un prodotto, materiale, oggetto, ecc.). In particolare, basandosi su un'impostazione bayesiana, il documento spiega come modellizzare e calcolare i rischi specifici e globali del consumatore e del produttore. In questo lavoro, la metodologia viene generalizzata ad oggetti multicomponente (in cui, per ciascuna componente, la relativa grandezza di interesse deve essere valutata se conforme o meno ai rispettivi requisiti), e per un insieme di N oggetti estratti da una stessa popolazione (occorre calcolare la probabilità che in quel campione ci sia un certo numero desiderato di oggetti conformi).*

Key words: conformity assessment, consumer's and producer's risk, multicomponent items, finite sample.

[1] Francesca Pennecchi, Istituto Nazionale di Ricerca Metrologica (INRIM); email: f.pennecchi@inrim.it

Ilya Kuselman, Independent Consultant on Metrology, 4/6 Yarehim St., 7176419 Modiin, Israel; email: ilya.kuselman@bezeqint.net

Francesca Pennecchi and Ilya Kuselman

1 The JCGM 106:2012 approach for conformity assessment

According to the definition of the JCGM 106:2012 document [5] "conformity assessment is any activity undertaken to determine, directly or indirectly, whether a product, process, system, person or body meets relevant standards and fulfils specified requirements". The document provides guidance and procedures for assessing the conformity of an item (entity, object or system).

The conformity assessment (CA) of an item of interest, such as a gauge block of an industrial production or a sample of air from an environment under air quality control, requires to check whether a certain property of interest of the item, i.e., the measurand [6, Sec. 2.3] (e.g., the length of the gauge block or the concentration of a specific pollutant within the air sample), lies within a prescribed tolerance interval (TI). In general, however, the true value η of the measurand is never completely known but it needs to be measured. Hence, CA decisions such as "the item is conforming" or "the item is rejected" rely on a measured value η_m, which has always a measurement uncertainty (MU) [4] associated with it. The accept/reject decision is based on the evidence of η_m falling or not, respectively, in an acceptance interval (AI) of permissible measured values. AI can differ from TI, in a way to favour either the consumer's or the producer's interests, and is typically established by taking into account the value of MU associated with η_m.

In order to use all available knowledge on the measurand, a Bayesian modelling is considered for the measurable quantity Y: the pre-measurement information is represented by a prior pdf $g_0(\eta)$, whereas the post-measurement state of knowledge is modelled by the posterior pdf $g(\eta|\,\eta_m)$, which is given by the following expression:

$$g(\eta|\,\eta_m) = C\, g_0(\eta)\, h(\eta_m|\,\eta), \tag{1}$$

where C is a normalizing constant and $h(\eta_m|\,\eta)$ is the likelihood function of η given η_m, that is the pdf of possible η_m values of the measuring system output quantity Y_m, at the true value $Y = \eta$ of the measurand.

Based on eq. (1), the following risks of erroneous decisions can be defined and calculated for both the consumer (probability of accepting the item, when it should have been rejected) and the producer (probability of falsely rejecting the item), respectively:

- Specific risks (for a specific item)

$$R_c^* = \int_{TI'} g(\eta|\,\eta_m)\, d\eta \text{ for a specific } \eta_m \text{ in AI}, \tag{2}$$

$$R_p^* = \int_{TI} g(\eta|\,\eta_m)\, d\eta \text{ for a specific } \eta_m \text{ in AI'}. \tag{3}$$

- Global risks (for an item to be chosen at random from the production process)

$$R_c = \int_{TI'} \int_{AI} g_0(\eta)\, h(\eta_m|\,\eta)\, d\eta_m\, d\eta, \tag{4}$$

$$R_p = \int_{TI} \int_{AI'} g_0(\eta)\, h(\eta_m|\,\eta)\, d\eta_m\, d\eta. \tag{5}$$

In eqs. (2-5), TI' and AI' indicate the set of true and measured values which lies outside TI and AI, respectively. Eqs. (2-3) involve integration of the posterior pdf (1), whereas eqs. (4-5) are double integrals of the joint pdf $f(\eta, \eta_m) = g_0(\eta)\ h(\eta_m|\ \eta)$ of variables Y and Y_m.

2 Generalization to multicomponent items

The JCGM 106 "deals with items having a single scalar property with a requirement given by one or two tolerance limits" and states: "the concepts presented can be extended to more general decision problems". For example, when, for each item, more than one measurable quantity should undergo CA (like in the case of several properties of a blood sample in a routine blood analysis), the CA would be performed separately for every parameter of interest. However, when CA for each particular component is successful and particular consumer and producer's risks (2-5) are acceptable, the total probability of a false decision on the conformity of the material as a whole might still be significant.

The IUPAC projects [1, 2] and corresponding IUPAC/CITAC Guide [7], addressed this topic by defining and modelling total consumer's risks and producer's risks (both specific and global):

- $R^*_{\text{total(c)}}$ is the probability that a specific accepted item[1] does not conform, as a whole, i.e., the true value of at least one component is not conforming;
- $R^*_{\text{total(p)}}$ is the probability that the true values of all components in a specific rejected item[2] are conforming;
- $R_{\text{total(c)}}$ is the probability that an item with a non-conforming true value of one or more components will be accepted based on a statistical analysis of performed measurement results;
- $R_{\text{total(p)}}$ is the probability that an item with conforming true values of all the components will be rejected based on a statistical analysis of performed measurement results.

The current project [3] "Influence of a mass balance constraint on uncertainty of test results of a substance or material and risks in its conformity assessment", is tackling the CA of compositional (multicomponent) items, whose components are linked by a mass balance constraint.

2.1 Total risks for independent variables

[1] A multicomponent item is accepted if the measured value of each component lays in its own acceptance interval.

[2] A multicomponent item is rejected when the measured value of at least one of the components lays outside its own acceptance interval.

When the measurable quantities Y_i and the measuring system output quantities $Y_{i\mathrm{m}}$ are independent, component by component i, it can be demonstrated, based on the law of total probability, that the total specific risks $R^*_{\mathrm{total(c,p)}}$ are a combination of particular specific ones (2) or (3), respectively [7]. For example, for just two components under CA, $R^*_{\mathrm{total(c)}} = R_{1\mathrm{c}}^* + R_{2\mathrm{c}}^* - R_{1\mathrm{c}}^* R_{2\mathrm{c}}^*$. Total global risks $R_{\mathrm{total(c,p)}}$ result instead in a combination of particular global risks (4) or (5), weighted by probabilities $\mathrm{P}(C_i) = \mathrm{P}(Y_{i\mathrm{m}}$ in $\mathrm{AI}_i)$ [7]. For two components under CA, for example, one has $R_{\mathrm{total(c)}} = \mathrm{P}(C_2)\, R_{1\mathrm{c}} + \mathrm{P}(C_1)\, R_{2\mathrm{c}} - R_{1\mathrm{c}}\, R_{2\mathrm{c}}$.

A case study on the monitoring total suspended particulate matter (TSPM) in ambient air, where pollutant concentrations caused by three stone quarries were taken as independent, showed a total global risk higher than the three particular ones.

2.2 Total risks for correlated variables

When correlations are present among measurable quantities Y_i and/or measuring system output quantities $Y_{i\mathrm{m}}$, for $i = 1, \ldots, n$, a multivariate Bayesian approach is adopted, involving multivariate pdfs and likelihood functions:

$$g(\boldsymbol{\eta}|\, \boldsymbol{\eta}_\mathrm{m}) = C\, g_0(\boldsymbol{\eta})\, h(\boldsymbol{\eta}_\mathrm{m}|\, \boldsymbol{\eta}), \tag{6}$$

where $\boldsymbol{\eta}$ and $\boldsymbol{\eta}_\mathrm{m}$ are the vectors of true and measured values of the components, respectively. In this case, the total specific risks are [7]:

$$R^*_{\mathrm{total(c)}} = 1 - \int_{\mathbf{TI}} g(\boldsymbol{\eta}|\, \boldsymbol{\eta}_\mathrm{m})\, \mathrm{d}\boldsymbol{\eta} \quad \text{for a specific } \boldsymbol{\eta}_\mathrm{m} \text{ in } \mathbf{AI}, \tag{7}$$

$$R^*_{\mathrm{total(p)}} = \int_{\mathrm{TI1}} \ldots \int_{\mathrm{TI}\nu} \int_{\mathrm{R}} \ldots \int_{\mathrm{R}} g(\boldsymbol{\eta}|\, \boldsymbol{\eta}_\mathrm{m})\, \mathrm{d}\boldsymbol{\eta} \quad \text{for a specific } \boldsymbol{\eta}_\mathrm{m} \text{ outside } \mathbf{AI}, \tag{8}$$

where $\mathbf{AI} = [\mathrm{AI}_1 \times \ldots \times \mathrm{AI}_n]$, $\mathbf{TI} = [\mathrm{TI}_1 \times \ldots \times \mathrm{TI}_n]$, the integral in eq. (7) is a multiple one, and $\boldsymbol{\eta}_\mathrm{m}$ in eq. (8) is outside $\mathbf{AI}$ at the first $\nu \le n$ components.

The total global risks are [7]:

$$R_{\mathrm{total(c)}} = \int_{\mathbf{TI'}} \int_{\mathbf{AI}} g_0(\boldsymbol{\eta})\, h(\boldsymbol{\eta}_\mathrm{m}|\, \boldsymbol{\eta})\, \mathrm{d}\boldsymbol{\eta}_\mathrm{m}\, \mathrm{d}\boldsymbol{\eta}, \tag{9}$$

$$R_{\mathrm{total(p)}} = \int_{\mathbf{TI}} \int_{\mathbf{AI'}} g_0(\boldsymbol{\eta})\, h(\boldsymbol{\eta}_\mathrm{m}|\, \boldsymbol{\eta})\, \mathrm{d}\boldsymbol{\eta}_\mathrm{m}\, \mathrm{d}\boldsymbol{\eta}, \tag{10}$$

where the multiple integration with respect to $\boldsymbol{\eta}$ on **TI'** in eq. (9) addresses all those cases in which at least one true value η_i is outside its TI_i, whereas the multiple integration with respect to $\boldsymbol{\eta}_\mathrm{m}$ on **AI'** in eq. (10) addresses all those cases in which at least one measured value $\eta_{i\mathrm{m}}$ is outside its AI_i.

A case study on CA of a four-component alloy showed the impact of correlation among the components on the total risk: neglecting correlations would lead to an overestimation of the global consumer risk.

2.3 Total risks for compositional data

When the components of a multicomponent item are subject to a mass balance constraint, e.g. $\Sigma\eta_i$ = 100 %, they are intrinsically correlated. A so-called 'spurious' correlation is then observed in addition to other possible natural and/or technological correlations. Moreover, when choosing an appropriate prior pdf, the constraint for the true values of each component to lay in the domain [0, 100] % has to be taken into account. An approach based on Monte Carlo simulations from a multivariate truncated normal pdf followed by a closure operation was applied to a case study on the CA of a specific sausage product, made of four components (fat, protein, moisture, salt) [8].

3 Extension to a finite sample of items

A further direction toward which the JCGM 106 framework could be extended is the CA of a finite sample of *N* items drawn from a common population ("The concepts presented can be extended to more general conformity assessment problems based on measurements of a set of scalar measurands" [5]). The idea is related to CA of a sample of *N* units from a population, e.g., a batch of *N* items from a population of batches at a factory, producing such batches continuously, where each item should be tested (the item parameters are to be measured). This may be necessary in an aircraft, military or car industry, in clinical analysis of a group from a population (schoolers of a specific school, bus drivers of a specific company, chemists of a laboratory, etc), in assessing the results of air monitoring in a specific region, etc.

Therefore, a recent research activity aims at generalization of specific and global risks (2-5) for a sample of items, that is, at answering the following two questions, respectively:

1) Given a sample of *N* measured items (each characterized by specific risks (2-3)), among which *K* have been measured within their AI (good measured values - GMV), which is the probability that at least *J* of the *N* corresponding true values were actually conforming – or, equivalently, the probability that less than *J* true values were non-conforming (bad true values - BTV)?
2) Considering to randomly drawing a sample of *N* items from a population already characterized by global risks (4-5), which is the probability to have, among them, exactly K_1 that are GMV&BTV, K_2 that are BMV&GTV, K_3 that are GMV&GTV and K_4 that are BMV&BTV? Notice that K1 + K_2 + K_3 + K_4 = N.

3.1 Specific risk

In order to answer question 1) above, we can resort to a discrete random variable (r.v.) V counting, among N, how many of the measured values $\eta_{i\mathrm{m}}$ (where $i = 1, \ldots, N$ is now the index enumerating the items in the sample) actually come from a corresponding good true value η_i. V is then the sum of N independent Bernoulli r.v., each with its own success probability P(Y_i in TI | $\eta_{i\mathrm{m}}$), which is equal to 1 - $R_{i\mathrm{c}}$*, if $\eta_{i\mathrm{m}}$ is a GMV, or to $R_{i\mathrm{p}}$*, if $\eta_{i\mathrm{m}}$ is a BMV.

Therefore, considering question 1):

- V ~ Poisson binomial(1 - $R_{1\mathrm{c}}$*, …,1 - $R_{K\mathrm{c}}$*, $R_{(K+1)\mathrm{p}}$*,…, $R_{N\mathrm{p}}$*),
- and the answer is given by P($V \geq J$) (which is also equal to 1 - P($V < J$)).

Setting the desired[1] probability P($V \geq J$) leads to the solution of the inverse problem "which is the maximum J value allowing to reach the desired probability to actually have at least J good true values in that sample?".

3.2 Global risk

In order to answer question 2) in Sec. 3, let us consider that P(GMV&BTV) = R_c and P(BMV&GTV) = R_p, by definition, whereas

$$\mathrm{P(GMV\&GTV)} = \int_{\mathrm{TI}} \int_{\mathrm{AI}} g_0(\eta)\, h(\eta_\mathrm{m}|\, \eta)\, \mathrm{d}\eta_\mathrm{m}\, \mathrm{d}\eta, \quad (11)$$

$$\mathrm{P(BMV\&BTV)} = \int_{\mathrm{TI'}} \int_{\mathrm{AI'}} g_0(\eta)\, h(\eta_\mathrm{m}|\, \eta)\, \mathrm{d}\eta_\mathrm{m}\, \mathrm{d}\eta. \quad (12)$$

Expressions (11) and (12) provide, in terms of a confusion matrix notation, the (probability of) true positives (p_TP) and true negatives (p_TN), respectively. Therefore, the discrete r.v. W able to answer question 2) has a multinomial pmf with parameters N and the probabilities provided by eqs. (4-5) and (11-12):

- W ~ multinomial(N; R_c, R_p, p_TP, p_TN) (Note that $R_\mathrm{c} + R_\mathrm{p} + p_\mathrm{TP} + p_\mathrm{TN} = 1$),
- and the answer is given by P($W = [K_1, K_2, K_3, K_4]$).

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[1] A requirement might be, for example, to reach at least 90 % probability of having at least 90 % of conforming items in the sample.

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