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A modified chi-square statistics of the linear estimator for inter-laboratory comparison

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A B S T R A C T

Chi-square statistics of the uncertainty weighted mean, which is a linear estimator, is widely used in data analysis of inter-laboratory comparison. However, the chi-square statistics of other linear estimators is not investigated. In this study, a modified chi-square statistics, which comprises the linear estimator, is proposed under the condition that comparison results are Gaussian distributed with a common mean. The proposed statistics is analyzed through Monte Carlo simulation by combining the weights of linear estimator into a multi-dimension vector. Simulation results show that the proposed statistics is $(n-1)$ th-order chi-square distributed when the weights vector of linear estimator is located in a particular subspace, which is influenced by the uncertainties of participants. Furthermore, this chi-square statistics of arithmetic mean is applied to the common mean and random effects models as examples. For the common mean model, the statistics can be applied to the hypothesis testing of arithmetic mean; for the random effects model, the statistics can be applied to the variance estimation of random effects.

1. Introduction

The traditional traceability system is strengthened by the signature of the CIPM Mutual Recognition Arrangement (MRA) [1–3]. The key comparison and its data analysis methods, which can be applied to a common inter-laboratory comparison, have been extensively studied as the technical basis of the MRA in recent years.

From the perspective of a statistical model, the data analysis methods are generally classified into common mean model (CMM) [4–6], random effects model (REM) [6] and fixed effects model (FEM) [6,7]. The CMM and REM assume that the comparison results of participants are Gaussian distributed with a common mean. Moreover, the chi-square statistics of uncertainty weighted mean is established in both models.

The CMM is the fundamental model. If n participants are involved in a comparison, then the result of ith participant is x_i, which is associated with the standard uncertainty u_i. The CMM can be expressed as

$$x_i = \mu + \varepsilon_i, \tag{1}$$

where μ is the measurand, ε_i is the random variable of the measurement error, and $\varepsilon_i \sim N(0, {u_i}^2)$ [6]. In addition, the comparison results of all participants are mutually independent. Under the conditions of the CMM, the uncertainty weighted mean is $x_w = \sum_{i=1}^{n} w_i \cdot x_i$, where the weight is $w_i = \frac{1}{{u_i}^2} \cdot \left(\sum_{i=1}^{n} \frac{1}{{u_i}^2}\right)^{-1}$. Furthermore, the $(n-1)$th-order chi-square statistics of x_w is

$$\chi^2_{obs} = \sum_{i=1}^{n} \frac{(x_i - x_w)^2}{{u_i}^2}, \tag{2}$$

which can be applied to the consistency testing of a comparison [4,8].

In the REM, random effects are added to the comparison results as

$$x_i = \mu + b_i + \varepsilon_i, \tag{3}$$

where b_i is the random effect, and $b_i \sim N(0, \tau^2)$. Therefore, the uncertainty of the ith participant is changed to $u^2(x_i) = \tau^2 + {u_i}^2$, by which the uncertainty weighted mean of the REM is obtained as x_w^{REM}. Similarly, the $(n-1)$th-order chi-square statistics of x_w^{REM} is

$$\chi^2_{REM} = \sum_{i=1}^{n} \frac{(x_i - x_w^{REM})^2}{\tau^2 + {u_i}^2}. \tag{4}$$

If the comparison results and uncertainties are known, then τ^2 can be estimated on the basis of $\mathrm{E}(\chi^2_{REM}) = n-1$ and moment estimation method [9,10]. For example, Mandel-Paule [9,11] and DerSimonian-Laird [5,9] are two specific methods.

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Nomenclature

a	Expected value of $\chi^2_\gamma|_\gamma$
$\boldsymbol{a}$, $\boldsymbol{w}$ and $\boldsymbol{\gamma}$	Weights vectors of $\bar{x}$, x_w and x_γ
b	Random effect
D	Difference between maximum and minimum of curves deviation
E	Expected value
$\boldsymbol{S}_1$	A simulated sample of $\boldsymbol{\gamma}$
u_i	Standard uncertainty of ith participant
Var	Variance
w_i	Weight of x_i in x_w
x_i	Comparison result of ith participant
x_w and x_w^{REM}	Uncertainty weighted means in common mean model and random effects model
$\bar{x}$	Arithmetic mean
x_γ	Linear estimator
y_j	jth value generated from 0 to 1 uniform distribution

Greeks

χ^2_{obs} and χ^2_{REM}	Chi-square statistics for x_w in common mean model and random effects model
χ^2_γ	Chi-square statistics for x_γ
ε_i	Measurement error of ith participant
μ	Measurand
γ_i	Weight of x_i in x_γ
τ^2	Variance of random effects

Conditions

$|_\gamma$	γ is fixed
$|_{\gamma=}$	γ is fixed at a particular weights vector
$|_{n=2}$	Two participants in a comparison
$|_{u,n\geq 3}$	Three or more participants in a comparison and uncertainties equal to each other

The linear estimator [12] of an inter-laboratory comparison is

$$x_\gamma = \sum_{i=1}^{n} \gamma_i \cdot x_i, \tag{5}$$

where the weight is denoted by γ_i and in the scale of $0 < \gamma_i < 1$ with the constraint $\sum_{i=1}^{n}\gamma_i = 1$. Based on $\sum_{i=1}^{n}\gamma_i = 1$, we hold that $\mathrm{E}(x_\gamma) = \mu$; that is, x_γ is unbiased estimator of μ. However, if the x_w and x_w^{REM} are replaced by x_γ, then χ^2_{obs} and χ^2_{REM} are not chi-square distributed; further, the density also do not have an evident regularity [8], thereby resulting in unsuitable current chi-square statistics for other linear estimators, especially the arithmetic mean, which is a classical estimator [13].

In this study, a modified chi-square statistics of the linear estimator is proposed and analyzed through Monte Carlo simulation. Furthermore, the chi-square statistics of the arithmetic mean is applied to the CMM and REM as examples.

2. Modified chi-square statistics and properties

The analysis of a linear estimator is converted into an analysis of the combination of weights because the linear estimator is accordant with the weights. Owing to this viewpoint, the weights of a linear estimator are combined into a multi-dimension vector, which is denoted by $\boldsymbol{\gamma} = (\gamma_1, \cdots, \gamma_n)^T$, and the basic space of this weights vector is $0 < \gamma_i < 1$ and $\sum_{i=1}^{n}\gamma_i = 1$ according to (5). In addition, the weights vector of x_w is denoted by $\boldsymbol{w} = (w_1, w_2, \cdots, w_n)^T$, and the weights vector of $\bar{x}$ is denoted by $\boldsymbol{a} = (1/n, \cdots, 1/n)^T$.

According to (A1) in Appendix, χ^2_{obs} can be expressed as

$$\chi^2_{obs} = (n-1)\cdot\frac{\sum_{i=1}^{n} w_i\cdot(x_i - x_w)^2}{E\left(\sum_{i=1}^{n} w_i(x_i - x_w)^2\right)} = (n-1)\cdot\frac{\sum_{i=1}^{n} w_i\cdot(x_i - x_w)^2}{\sum_{i=1}^{n} w_i\cdot u_i^2 - \sum_{i=1}^{n} w_i^2\cdot u_i^2} \tag{6}$$

The modified chi-square statistics, which comprise the linear estimator x_γ, is proposed by replacing w_i by γ_i, as follows:

$$\chi^2_\gamma = (n-1)\cdot\frac{\sum_{i=1}^{n} \gamma_i\cdot(x_i - x_\gamma)^2}{\sum_{i=1}^{n} \gamma_i\cdot u_i^2 - \sum_{i=1}^{n} \gamma_i^2\cdot u_i^2} \tag{7}$$

This statistics is analyzed in the CMM which is a simple model, and then is extended to the REM as an application example in Section 5.

Under the conditions of the CMM, the properties of χ^2_γ are listed as follows:

Property 1. *Based on $x_i = \mu + \varepsilon_i$ and $x_\gamma = \mu + \sum_{i=1}^{n}\gamma_i\cdot\varepsilon_i$, we hold that $x_i - x_\gamma = \varepsilon_i - \sum_{i=1}^{n}\gamma_i\cdot\varepsilon_i$, in which μ is eliminated. In other words, the distribution of χ^2_γ is unaffected by the value of μ.*

Property 2. *If $\boldsymbol{\gamma}$ is fixed (which is constant but not variable) in the basic space, then we hold that $\mathrm{E}\left(\chi^2_\gamma|_\gamma\right) = n - 1$ in the CMM and REM. (Appendix)*

Property 3. *If $\boldsymbol{\gamma} = \boldsymbol{w}$, then we hold that $\chi^2_\gamma|_{\gamma=\boldsymbol{w}} = \chi^2_{obs}$, which means $\chi^2_\gamma|_{\gamma=\boldsymbol{w}}$ is (n - 1)th-order chi-square distributed.*

Property 4. *If $\boldsymbol{\gamma}\neq\boldsymbol{w}$, then $\chi^2_\gamma|_\gamma$ is possibly (n - 1)th-order chi-square distributed. For example, if $\boldsymbol{\gamma} = \boldsymbol{a}$, then (7) is derived as*

$$\chi^2_\gamma|_{\gamma=\boldsymbol{a}} = n\cdot\frac{\sum_{i=1}^{n}\left(x_i - \bar{x}\right)^2}{\sum_{i=1}^{n} u_i^2}, \tag{8}$$

and this equation is a statistics of arithmetic mean $\bar{x}$. In addition, four participants are involved in an inter-laboratory comparison, and comparison results are Gaussian distributed with the uncertainties 1.4, 2.0, 1.6 and 1.8 for the four participants. Then, the Monte Carlo simulation is adopted to analyzed the distribution of $\chi^2_\gamma|_{\gamma=\boldsymbol{a}}$. Based on Property 1, μ is valued by 0 during the simulation [8]. The simulation procedures are summarized as follows:

① According to $N(0, u_i^2)$, n groups of x_i $(i = 1\cdots n)$ samples are generated for each participant, and the samples number of a group is 10^6.
② In accordance with (7) and (8), two groups, that is $\chi^2_\gamma|_{\gamma=\boldsymbol{w}}$ and $\chi^2_\gamma|_{\gamma=\boldsymbol{a}}$ samples, are calculated by the same samples of x_i and different weight vectors $\boldsymbol{w}$ and $\boldsymbol{a}$.
③ The simulated density curves of $\chi^2_\gamma|_{\gamma=\boldsymbol{w}}$ and $\chi^2_\gamma|_{\gamma=\boldsymbol{a}}$ are obtained from the histogram method.

In Fig. 1, the simulated curves are in accordance with the exact curve of the third-order chi-square; that is, $\chi^2_\gamma|_{\gamma=\boldsymbol{w}}$ and $\chi^2_\gamma|_{\gamma=\boldsymbol{a}}$ are