# Intervals of confidence on nested standard deviations

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**Abstract:**

In many situations, standard deviations (SD) need to be computed from a nested design. This typically happens in procedures of quality control and in laboratory inter-comparisons. In such situations, the basics for computing SD is well known but existing methods to compute the interval of confidence (IC) on them are rather unsatisfactory. In particular, they fail totally to account negative values that are often encountered for corresponding estimated variances. This article provides equations that describe well the distributions of variances of nested levels and their scatter, provided that the true values of them is known. Both cases of 2 nested levels and more than 2 nested levels are considered. Inversing them to find out IC on true values of variances as function of their estimations is unfortunately impossible when variances of lower levels are unknown. However, this article proposes approaching equations that can be used when the impact of the variances of lower levels can be expected to be low. Methods to check whether this condition is fulfilled are also proposed. When not, the numbers of repetitions at the lower levels need to be increased to get an acceptable determination of the IC.

# 1 Introduction

In many situations, standard deviations need to be computed from a nested design. This typically happens in laboratory proficiency testing when the interlaboratory SD (standard deviation) or the homogeneity SD is computed from a series of repeated tests. It also happens in many other situations, for example when a long-term quality level of a production is computed from a series of release test results.

In such situations, the basics for computing SD is well known but existing methods to compute the IC on them are rather unsatisfactory. In particular, they fail totally to account negative values that are often encountered for corresponding estimated variances.

This document provides:

- Examples where such IC are needed;
- Technical backgrounds of calculations of them for 2 levels and more than 2 levels;
- Approached formulas to compute IC on estimated nested variances when the ratio of nested variances is known;
- Methods to compute IC on estimated nested variances when the ratio of nested variances is unknown.

# 2 Symbols and abbreviations

The symbols used in this document are listed in Table 1.

*Table 1. List of symbols used in this document.*

| ***Symbol*** | **Designation and comments** |
|---|---|
| ***i*** | Level of nested variances (levels are ordered from the inside to the outside of the design of experiments) |
| ***j*** | Index inside a given *i* level |
| ***k*** | Total number of nested levels |
| $m_1$ | Mean value of $x_{1,j}$ ($m_1 = \sum x_j / n_1$) |
| $m_i$ | Mean value of $m_{i-1}$ values ($m_i = \sum m_{i-1} / n_i$) |
| $sd_i$ | Estimate of $SD_i$ |
| $SD_i$ | Standard deviation of level *i* |
| ***T*** | Threshold value for $V_1/(n_1.V_2)$ associated with an $\alpha$ value for the IC and with the parameters $n_1$, $n_2$, $V_1$ and $V_2$ for which the lower limit of the IC on $v_2$ is negative |
| $v_i$ | Estimate of $V_i$ |
| $V_i$ | Variance of level *i* ($V_i = SD_i^2$) |
| $w_i$ | Global variance of level *i*, as defined in Equation (1) and Equation (7) |
| $x_{ij}$ | Basic values from which $m_i$ and $sd_i$ are computed |
| ***α*** | Level of confidence for intervals of confidence |

Abbreviations:

- IC: bilateral interval of confidence. For example, IC95% means the bilateral interval of confidence [2,5%;97,5%]
- MCM: Monte-Carlo method
- PT: proficiency tests
- SD: standard deviation

# 3 Examples where an IC on a nested SD may be needed

Each time that a SD is computed from a series of series of repeated results, the knowledge of the corresponding IC may be needed. This happens for example in the following situations:

- Attestation of conformity on the basis of long-term quality level, as specified for example in EN 10080 [1]. The quality level of the product (in this case, reinforcing steels for concrete) is attested not only by release tests and external tests, but also by a surveillance of the long-term quality level of the production of the factory. For achieving this, a long-term SD of the produced batches is computed from the series of release tests. The internal SD of batches needs to be taken into account to get this long-term SD of production;
- Precision test experiments specified in ISO 5725-2 [2] are based on ANOVA (analysis of variances) which decomposes nested SD corresponding to the different levels of precision (typically repeatability, intermediate levels and reproducibility). The computation of intermediate precision SD may then request to take into account sub-level SD;
- In PT as specified in ISO 13528 [3], the check of homogeneity of items used for PT (as described in annex B) requests to take into account the SD of repeatability of tests used to achieve this check;

- In both upper cases, more than 2 levels may occur, for example, level 1 is repetition of tests in repeatability conditions, level 2 is repetition of tests on different samples, level 3 is repetition of tests using different operators, equipment and periods of time and level 4 involves test results from several laboratories.

# 4 Basics for the estimation of a variance with nested levels

## 4.1 Classical methods for 2 nested levels

The basic equation for computing a variance with 2 nested levels is reminded in Equation (1):

$$v_2 = w_2 - v_1/n_1 \qquad (1)$$

*Where $v_2$ is the estimate of $V_2$,*

$$w_2 = \left( \sum_{1}^{n_2} (m_{1j} - m_2)^2 \right) \Big/ (n_2 - 1)$$

*$v_1$ is the estimate of $V_1$,*

*and $n_1$ is the number of results used to compute $v_1$.*

***Example 1:***

*In a check of homogeneity of samples in accordance with annex B of ISO 13528 [3], test results of Table 2 were found.*

*Table 2. Example of calculation of $w_2$.*

| | Sample 1 | Sample 2 | Sample 3 | Sample 4 | Sample 5 | Sample 6 | Sample 7 | Sample 8 | Sample 9 | Sample 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| **Test 1** | 103,2 | 99,6 | 99,3 | 100,6 | 101,7 | 101,6 | 97,1 | 97,7 | 106,8 | 97,4 |
| **Test 2** | 99,8 | 96,5 | 100,7 | 100,6 | 100,4 | 105,1 | 99,4 | 101,3 | 102,4 | 97,8 |
| $m_{1j}$ | 101,5 | 98,05 | 100 | 100,6 | 101,05 | 103,35 | 98,25 | 99,5 | 104,6 | 97,6 |
| $v_{1j}$ | 5,78 | 4,805 | 0,98 | 0 | 0,845 | 6,125 | 2,645 | 6,48 | 9,68 | 0,08 |

*Then,* $w_2 = \sum_{j=1}^{10} m_{1j}/10 = 5{,}216$, $v_1 = \sum_{j=1}^{10} v_{1j}/10 = 3{,}742$, $n_1 = 2$, $v_2 = 5{,}216 - 3{,}742/2 = 3{,}345$

Several ways are classically proposed to compute the IC on $V_2$ as for example:

- In [4], IC is computed with the equation $IC = (w_2.F)/n_1$ where F is the Fisher Snedecor value (depending on $n_1$, $n_2$ and α). In this example, the IC90% would then be [-1,74;0,61];
- IC may also be computed with the equation $IC = (w_2 - v_1/n_1)/\chi^2_{\alpha,n_2-1}$. In this example, the IC90% would then be [1,24;6,29].

Unfortunately, none of them fits the MCM simulations (see [5]). In particular, they do not cope well with negative results often found, in particular the second option. This is because, in both cases, more or less only one source of scatter is taken into account instead of two. This is particularly obvious in the second case, where the quantity $w_2 - v_1/n_1$ plays the same role than s² in simple variance estimation according to Equation (2) (origin: ISO 2854 [6]).

$$(n-1).\frac{v}{V} \approx \chi^2_{n-1} \qquad (2)$$

## 4.2 Estimation of a variance with 2 nested levels

We could verify with the MCM that Equation (3), equivalent to Equation (2), describes exactly the distribution of estimates of variances with 2 nested levels.

$$\frac{v_2}{V_2} \approx \left(1+\frac{V_1}{n_1.V_2}\right).\frac{\chi^2_{n_2-1}}{n_2-1} - \frac{V_1}{n_1.V_2}.\frac{\chi^2_{n_2.(n_1-1)}}{n_2.(n_1-1)} \quad (3)$$

*Note: When used in the MCM, this Equation (3) needs to be used with independent random α values for the two χ² functions. For this reason, it cannot be re-written in the form* $\frac{v_2}{V_2} \approx \frac{\chi^2_{n_2-1}}{n_2-1}.\left(1+\frac{V_1}{n_1.V_2}.\left(1-F_{n_2.(n_1-1),n_2-1}\right)\right)$ *because of covariance effects.*

*Note:* $V_2$*, which is the true variance cannot be negative, but* $v_2/V_2$ *obviously can, leading to negative values for* $v_2$*. In those cases,* $sd_2 = \sqrt{v_2}$ *cannot be computed and* $sd_2$ *is usually then regarded as equal to 0.*

*Note: As the mean value of a* $\chi^2$ *distribution is its number of degrees of freedom, we can easily verify that the mean value of the distribution described by Equation (3) is equal to 1. This confirms that Equation (3) provides estimates without bias of* $v_2/V_2$*.*

This Equation (3) rises the following comments:

**Comment 1:**

The first term Equation (3), i.e. $\left(1+\frac{V_1}{n_1.V_2}\right).\frac{\chi^2_{n_2-1}}{n_2-1}$ addresses the term $w_2$ of Equation (1) while the term $\frac{V_1}{n_1.V_2}.\frac{\chi^2_{n_2.(n_1-1)}}{n_2.(n_1-1)}$ of Equation (3) addresses the term $v_1/n_1$ of Equation (1).

**Comment 2:**

The term $V_1/(n_1.V_2)$ plays a fundamental role in the accuracy of the estimation of $v_2/V_2$:

- When $V_1/(n_1.V_2) \ll 1$, then $\frac{v_2}{V_2} \approx \frac{\chi^2_{n_2-1}}{n_2-1}$, that is to say a situation equivalent to Equation (2);
- When $V_1/(n_1.V_2) \gg 1$, then $\frac{v_2}{V_2} \approx \frac{V_1}{n_1.V_2}.\left(\frac{\chi^2_{n_2-1}}{n_2-1} - \frac{\chi^2_{n_2.(n_1-1)}}{n_2.(n_1-1)}\right)$, i.e. a random value in the range of $[-k.V_1/(n_1.V_2); +k.V_1/(n_1.V_2)]$, $k$ depending on $n_1$ and $n_2$, (see Equation (4) further on), and no valuable estimation of $v_2/V_2$ can be computed;
- The situations where $V_1/(n_1.V_2) \cong 1$ are intermediate, where estimations of $v_2/V_2$ can be computed, but they may be of poor quality.

**Comment 3:**

Equation (3) involves a combination of 2 independent random values (i.e. $\chi^2_{n_2-1}$ and $\chi^2_{n_2.(n_1-1)}$). Unfortunately, if a sum of two $\chi^2$ is easy to handle (from the definition of $\chi^2$), a difference of two $\chi^2$ is not at all.

However, as the variance of a $\chi^2_n$ distribution is *2n* and thanks to the law of combination of variances, we can easily compute the exact SD of the estimates of $v_2/V_2$ with Equation (4), as follows:

$$SD\left(\frac{v_2}{V_2}\right) = \sqrt{\left(1+\frac{V_1}{n_1.V_2}\right)^2.\frac{2}{n_2-1} + \left(\frac{V_1}{n_1.V_2}\right)^2.\frac{2}{n_2.(n_1-1)}} \quad (4)$$

Moreover, it could be confirmed with the MCM that the quadratic mean of the resulting distribution is equal to 1, confirming that Equation (3) provides an estimation without bias of $v_2/V_2$.

**Comment 4:**

In practice, the interesting ratio is $V_2/v_2$ and not $v_2/V_2$, because we know $v_2$ and we are looking for an IC on $V_2$. Getting an IC on *V* from *v* when using Equation (2) is easy, but getting an IC on $V_2$ from $v_2$ by using Equation (3) is not easy at all, and even impossible when the ratio $V_1/V_2$ is not known. We will come back to this issue at § 5.

**Comment 5:**

We could verify with the MCM that, even if Equation (3) produces asymmetric distributions, the quantiles $(v_2/V_2)_\alpha$ (where $\alpha$ is the cumulative probability of the distribution) are distributed such that values of differences $(v_2/V_2)_{1-\alpha} - (v_2/V_2)_\alpha$ are close to differences between corresponding quantiles of Gaussian distributions with same SD. For example, differences $(v_2/V_2)_{0,975} - (v_2/V_2)_{0,05} \cong 4.SD(v_2/V_2)$ as computed with Equation (4).

**Comment 6:**

In the same way, we could verify with the MCM that, even if Equation (3) produces asymmetric distributions, the central value for a given $\alpha$ value can be approached by the Equation (5) as follows.

$$CV_\alpha\left(\frac{v_2}{V_2}\right) \cong \left(1+\frac{V_1}{n_1.V_2}\right).\frac{\chi^2_{1-\alpha,n_2-1}+\chi^2_{\alpha,n_2-1}}{2.(n_2-1)} - \frac{V_1}{n_1.V_2}.\frac{\chi^2_{1-\alpha,n_2.(n_1-1)}+\chi^2_{\alpha,n_2.(n_1-1)}}{2.n_2.(n_1-1)} \qquad (5)$$

*Where* CV$_\alpha$ *represents a central value of the distribution of estimates of* $(v_2/V_2)_\alpha$ *for a given* α.

## 4.3 Equation to compute an approached value of *(v2/V2)α* for a given *α*

Comments 5 and 6 enable us to compute approached values of $(v_2/V_2)_\alpha$ using Equation (6), as follows:

$$(v_2/V_2)_\alpha = CV_\alpha + k_\alpha.SD \qquad (6)$$

*Where* CV$_\alpha$ *represents a central value of the distribution of estimates of* $(v_2/V_2)_\alpha$ *for a given* α*, computed with Equation* (5)*,*
k *is the quantile of the Gaussian distribution,*
SD *is the standard deviation of the distribution of estimates of the variance, computed with Equation* (4)*.*

***Example 2:***

*Scheme used in example 1, i.e.* $n_1 = 2$, $n_2 = 10$ *for which* $V_1/V_2$ *would be equal to 4 (i.e.* $SD_1 = 2.SD_2$*, which makes sense in the context of ISO 13528 annex B), and which was used to build up example 1. Then* $V_1/(n_1.V_2) = 2$, $SD\left(\frac{v_2}{V_2}\right) = \sqrt{(1+2)^2.\frac{2}{10-1}+(2)^2.\frac{2}{10.(2-1)}} \cong 1{,}673$ *and the subsequent calculations can be seen in Table* 3.

*Table 3. Example of calculation of an approached value of $(v_2/V_2)_\alpha$.*

| α | $(v_2/V_2)_\alpha$ **computed with the MCM** | $\frac{\chi^2_{\alpha,n_2-1}}{n_2-1}$ | $\left(\frac{\chi^2_{\alpha,n_2-1}}{n_2-1}+\frac{\chi^2_{1-\alpha,n_2-1}}{n_2-1}\right)/2$ | $\frac{\chi^2_{\alpha,n_2.(n_1-1)}}{n_2.(n_1-1)}$ | $\left(\frac{\chi^2_{\alpha,n_2.(n_1-1)}}{n_2.(n_1-1)}+\frac{\chi^2_{1-\alpha,n_2.(n_1-1)}}{n_2.(n_1-1)}\right)/2$ | $CV_\alpha\left(\frac{v_2}{V_2}\right)$ | k from Gaussian distribution | $(v_2/V_2)_\alpha = CV_\alpha + k.SD$ |
|---|---|---|---|---|---|---|---|---|
| 0,025 | **-2,02** | 0,300 | 1,207 | 0,325 | 1,187 | 1,248 | -1,960 | **-2,03** |
| 0,05 | **-1,54** | 0,369 | 1,125 | 0,394 | 1,112 | 1,149 | -1,645 | **-1,60** |
| 0,1 | **-1,00** | 0,463 | 1,047 | 0,487 | 1,043 | 1,057 | -1,282 | **-1,09** |
| 0,2 | **-0,36** | 0,598 | 0,979 | 0,618 | 0,981 | 0,975 | -0,842 | **-0,43** |
| 0,5 | **0,87** | 0,927 | 0,927 | 0,934 | 0,934 | 0,913 | 0,000 | **0,91** |
| 0,8 | **2,29** | 1,360 | 0,979 | 1,344 | 0,981 | 0,975 | 0,842 | **2,38** |
| 0,9 | **3,15** | 1,632 | 1,047 | 1,599 | 1,043 | 1,057 | 1,282 | **3,20** |
| 0,95 | **3,92** | 1,880 | 1,125 | 1,831 | 1,112 | 1,149 | 1,645 | **3,90** |
| 0,975 | **4,64** | 2,114 | 1,207 | 2,048 | 1,187 | 1,248 | 1,960 | **4,53** |

*Note that α are chosen so that values of tables can be found at the 1-α line. For example, for α = 0,025, $\frac{\chi^2_{1-\alpha,n_2-1}}{n_2-1} = 2{,}114$. Then, the term of the fourth column is $(0{,}300 + 2{,}114)/2 = 1{,}207$.*

*We can conclude from this table that, when $n_1 = 2$, $n_2 = 10$ and $SD_1/SD_2 = 2$, 95% of estimates $sd_2$ of the standard deviation $SD_2$ are included in the interval [0;2,13], about 35% of them being equal to 0.*

We can see from this example that Equation (6) provides not bad approached values for $(v_2/V_2)_\alpha$. Moreover, MCM simulations for a large number of $n_1$, $n_2$ and $V_1/V_2$ sets of values, Equation (6) turned out to be more accurate when either $V_1/(n_1.V_2) \ll 1$ or $V_1/(n_1.V_2) \gg 1$. In other words, this example for which $V_1/(n_1.V_2) \cong 1$ is not a favourable example.

As a conclusion, globally speaking, Equation (6) appeared to provide $(v_2/V_2)_\alpha$ values to the nearest 0,1 or 10%, the greatest of the two, and quite better when $V_1/(n_1.V_2)$ is not closed to 1 and/or when $n_1$ and/or $n_2$ are large. Moreover, when $n_1$ and/or $n_2$ are large, $\left(\frac{\chi^2_{\alpha,n_2-1}}{n_2-1}+\frac{\chi^2_{1-\alpha,n_2-1}}{n_2-1}\right)/2$ and $\left(\frac{\chi^2_{\alpha,n_2.(n_1-1)}}{n_2.(n_1-1)}+\frac{\chi^2_{1-\alpha,n_2.(n_1-1)}}{n_2.(n_1-1)}\right)/2$ become close to 1 whatever $\alpha$, and Equation (6) can be simplified into $(v_2/V_2)_\alpha = 1 + k_\alpha.SD$.

## 4.4 Estimation of a variance with more than 2 nested levels

In accordance with ANOVA principles, when more than 2 nested levels are used, Equations (1),(3) and (4) need to be extended into Equations (7) to (11) as follows:

Equation (7) is the extension of Equation (1), as follows:

$$v_i = w_i - \frac{v_{i-1}}{n_{i-1}} - \frac{v_{i-2}}{n_{i-1} \times n_{i-2}} - \cdots - \frac{v_1}{n_{i-1} \times n_{i-2} \times \ldots \times n_1} \tag{7}$$

*Where* i *is the rank of the considered level,*
*k is the total number of nested levels,*
$V_i$ *is the true variance of level* i*,*
$v_i$ *is the estimate of* $V_i$*,*
$w_i = \left(\sum_1^{n_2}(m_{ij} - m_i)^2\right)/(n_i - 1)$*,*
$n_i$ *is the total number of series of results used to compute* $v_i$*.*

Using algebraic transformations, Equation (7) can also be expressed as Equation (8) as follows, which allows to compute $v_i$ with no need to compute all $v_{i-1}$ to $v_1$ values before:

$$v_i = w_i - \frac{\sum Var(m_{i-2})}{n_k \times n_{k-1} \times \ldots \times n_{i-1}} \tag{8}$$

Equation (9) is the extension of Equation (3), as follows:

$$\begin{aligned}\frac{v_i}{V_i} \approx & \left(1 + \frac{V_{i-1}}{n_{i-1} \times V_i} + \frac{V_{i-2}}{n_{i-1} \times n_{i-2} \times V_i} + \cdots + \frac{V_1}{n_{i-1} \times n_{i-2} \times \ldots \times n_1 \times V_i}\right) \times \frac{\chi^2_{(n_i-1).n_{i+1}.n_{i+2}.\ldots.n_k}}{(n_i - 1) \times n_{i+1} \times n_{i+2} \times \ldots \times n_k} \\ & - \left(\frac{V_{i-1}}{n_{i-1} \times V_i} + \frac{V_{i-2}}{n_{i-1} \times n_{i-2} \times V_i} + \cdots + \frac{V_1}{n_{i-1} \times n_{i-2} \times \ldots \times n_1 \times V_i}\right) \times \frac{\chi^2_{n_k \times n_{k-1} \times \ldots \times (n_{i-1}-1)}}{n_k \times n_{k-1} \times \ldots \times (n_{i-1} - 1)}\end{aligned} \tag{9}$$

Equation (10) is the extension of Equation (4), as follows:

$$\begin{aligned}SD\left(\frac{v_i}{V_i}\right) = & \left(\left(1 + \frac{V_{i-1}}{n_{i-1} \times V_i} + \frac{V_{i-2}}{n_{i-1} \times n_{i-2} \times V_i} + \cdots + \frac{V_1}{n_{i-1} \times n_{i-2} \times \ldots \times n_1 \times V_i}\right)^2 \times \frac{2}{(n_i - 1) \times n_{i+1} \times n_{i+2} \times \ldots \times n_k}\right. \\ & \left. + \left(\frac{V_{i-1}}{n_{i-1} \times V_i} + \frac{V_{i-2}}{n_{i-1} \times n_{i-2} \times V_i} + \cdots + \frac{V_1}{n_{i-1} \times n_{i-2} \times \ldots \times n_1 \times V_i}\right)^2 \times \frac{2}{n_k \times n_{k-1} \times \ldots \times (n_{i-1} - 1)}\right)^{1/2}\end{aligned} \tag{10}$$

Equation (11) is the extension of Equation (5), as follows:

$$\begin{aligned}CV_\alpha\left(\frac{v_i}{V_i}\right) \cong & \left(1 + \frac{V_{i-1}}{n_{i-1} \times V_i} + \frac{V_{i-2}}{n_{i-1} \times n_{i-2} \times V_i} + \cdots + \frac{V_1}{n_{i-1} \times n_{i-2} \times \ldots \times n_1 \times V_i}\right) \\ & \times \frac{\chi^2_{1-\alpha,(n_i-1).n_{i+1}.n_{i+2}.\ldots.n_k} + \chi^2_{\alpha,(n_i-1).n_{i+1}.n_{i+2}.\ldots.n_k}}{2.(n_i - 1) \times n_{i+1} \times n_{i+2} \times \ldots \times n_k} \\ & - \left(\frac{V_{i-1}}{n_{i-1} \times V_i} + \frac{V_{i-2}}{n_{i-1} \times n_{i-2} \times V_i} + \cdots + \frac{V_1}{n_{i-1} \times n_{i-2} \times \ldots \times n_1 \times V_i}\right) \\ & \times \frac{\chi^2_{1-\alpha,n_k \times n_{k-1} \times \ldots \times (n_{i-1}-1)} + \chi^2_{\alpha,n_k \times n_{k-1} \times \ldots \times (n_{i-1}-1)}}{2.n_k \times n_{k-1} \times \ldots \times (n_{i-1} - 1)}\end{aligned} \tag{11}$$

We can see that the term $\frac{V_{i-1}}{n_{i-1}\times V_i}+\frac{V_{i-2}}{n_{i-1}\times n_{i-2}\times V_i}+\cdots+\frac{V_1}{n_{i-1}\times n_{i-2}\times\ldots\times n_1\times V_i}$ plays the same role than the term $V_1/(n_1.V_2)$ in the "2 level" case, and comments 1 and 2 of § 4.2 apply in the same way. It follows that the quality of estimation of $V_i$ depends on much more parameters than in the case of 2 levels. However, the number of degrees of freedom increases deeply when *i* decreases so that, in most cases, the influence of the variances of the lower levels is likely to be low.

As applications to these Equations:

- Example 3 describes the calculation of $v_i$ using Equation (8) in the case where 3 levels are nested and the IC of the variance of level 2 is searched. In this case, the approaching Equation (6) can be used with replacing $n_2$ with $n_2.n_3$;
- Example 4 describes the calculation of $v_i$ using Equation (8) in the case where more than 3 levels are nested;
- Example 5 describes the calculation of the centiles and the standard deviation of estimates of $v_i$ using Equations (9) and (10) in the case where more than 3 levels are nested.

***Example 3:***

*Let us consider the scheme used in example 1, that would be repeated 5 or 8 or 13 or 20 times (for example by 5 or 8 or 13 or 20 different laboratories). The subsequent calculations can be seen in Table 4.*

*Table 4. Example of calculation of variances of level 2 for 3 nested levels of variance.*

| | $(v_2/V_2)_\alpha$ computed with the MCM | | | | | $(v_2/V_2)_\alpha = CV_\alpha + k.SD$ | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **α** | $n_3=1$ | $n_3=3$ | $n_3=8$ | $n_3=13$ | $n_3=20$ | $n_3=1$ | $n_3=3$ | $n_3=8$ | $n_3=13$ | $n_3=20$ |
| **0,025** | -2,02 | -0,42 | -0,13 | 0,11 | 0,28 | -2,03 | -0,42 | -0,13 | 0,11 | 0,28 |
| **0,05** | -1,54 | -0,19 | 0,05 | 0,25 | 0,39 | -1,60 | -0,20 | 0,05 | 0,25 | 0,39 |
| **0,1** | -1,00 | 0,06 | 0,25 | 0,42 | 0,53 | -1,09 | 0,05 | 0,25 | 0,41 | 0,52 |
| **0,2** | -0,36 | 0,37 | 0,50 | 0,61 | 0,69 | -0,43 | 0,37 | 0,50 | 0,61 | 0,68 |
| **0,5** | 0,87 | 0,98 | 0,99 | 0,99 | 0,99 | 0,91 | 0,98 | 0,99 | 0,99 | 1,00 |
| **0,8** | 2,29 | 1,61 | 1,49 | 1,39 | 1,31 | 2,38 | 1,63 | 1,50 | 1,39 | 1,31 |
| **0,9** | 3,15 | 1,98 | 1,76 | 1,60 | 1,50 | 3,20 | 1,97 | 1,77 | 1,60 | 1,48 |
| **0,95** | 3,92 | 2,28 | 2,00 | 1,77 | 1,65 | 3,90 | 2,26 | 1,99 | 1,78 | 1,62 |
| **0,975** | 4,64 | 2,54 | 2,22 | 1,94 | 1,77 | 4,53 | 2,52 | 2,19 | 1,93 | 1,75 |

Unsurprisingly, the accuracy of determination of $V_2$ increases significantly when $n_3$is increasing.

***Example 4:***

*The MCM was used to determine IC95% of estimates of the standard deviation of homogeneity when $N_p$ is the number of participants, the number of samples per participant is 3 and the number of repetitions per sample is 2. Then, in this example, $n_3=N_p$, $n_2=3$, $n_1=2$, $V_2=\sigma_H^2$, $V_1=\sigma_r^2$. "Khi2 values" represent the IC when $V_1/(n_1.V_2)\to 0$.*

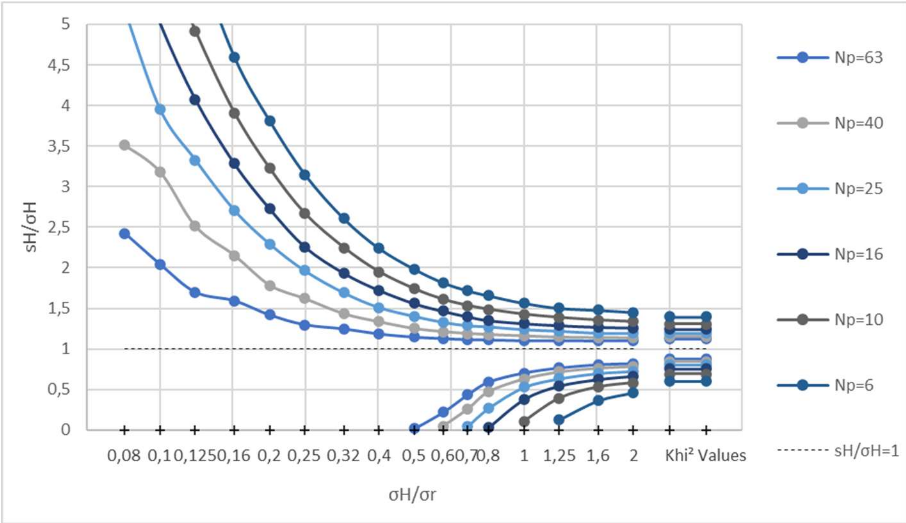


Figure 1: Lower and upper limits of the IC95% of $s_H/\sigma_H$ for $N_p$ participants, 3 samples per participant, 2 test results per sample.

*We can clearly see that there is a threshold value of $\sigma_H/\sigma_r$, i.e. $V_1/(n_1.V_2)$, under which $v_H$ may become negative and $s_H$ needs to be rounded to 0.*

When a variance of an intermediate level needs to be estimated, Equation (1) needs to be adapted as in the following example 5:

***Example 5:***

*Scheme used in example 1 with 5 levels for which $v_4$ needs to be estimated as shown in Table 4.*

*Table 5. Example of calculation of variance of level 4 with 5 nested levels with*
*$n_1 = 2$, $n_2 = 3$, $n_3 = 4$, $n_4 = 3$, $n_5 = 2$,*

| | | | Level 5 | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | | 1 | | | 2 | | |
| | | | Level 4 | | | | | |
| **Level 3** | **Level 2** | **Level 1** | **1** | **2** | **3** | **1** | **2** | **3** |
| 1 | 1 | 1 | 104,5 | 91,2 | 96 | 92,3 | 86,2 | 95,2 |
| 1 | 1 | 2 | 87 | 87,3 | 81,2 | 95,9 | 99,1 | 97,8 |
| 1 | 2 | 1 | 111,4 | 98,1 | 113,1 | 105,8 | 101,8 | 98,1 |
| **1** | **1** | **1** | 103,9 | 102 | 102,3 | 89,8 | 98,7 | 100,4 |
| **1** | **1** | **2** | 101,9 | 102,2 | 99,3 | 88,8 | 99 | 99,7 |
| **1** | **2** | **1** | 103,7 | 101,5 | 105,8 | 87,9 | 99,1 | 102 |
| **1** | **2** | **2** | 101,1 | 102,8 | 105,4 | 90,4 | 96,3 | 101,8 |
| **1** | **3** | **1** | 102,7 | 102 | 99,8 | 90,1 | 104,8 | 102,4 |
| **1** | **3** | **2** | 102,8 | 99,7 | 98,4 | 92 | 104,3 | 101,6 |
| **2** | **1** | **1** | 104,6 | 98,3 | 101,6 | 93,8 | 97,7 | 96,9 |
| **2** | **1** | **2** | 104,5 | 98,6 | 104,3 | 96,2 | 100,3 | 97,1 |
| **2** | **2** | **1** | 103,9 | 98,4 | 107,2 | 98,8 | 98,8 | 91,1 |
| **2** | **2** | **2** | 103,9 | 99,3 | 106,6 | 98,6 | 97,7 | 88,7 |
| **2** | **3** | **1** | 104 | 99,8 | 105,3 | 98,9 | 98,6 | 93,6 |
| **2** | **3** | **2** | 101,6 | 100,7 | 105,1 | 97,4 | 97,8 | 96,5 |
| **3** | **1** | **1** | 94,2 | 99,2 | 102,9 | 96,9 | 91,2 | 94,8 |
| **3** | **1** | **2** | 95,6 | 98,4 | 100,8 | 97 | 91,5 | 93,3 |
| **3** | **2** | **1** | 93,6 | 96 | 104,8 | 96,7 | 98 | 93,5 |

| | | | Level 5 | | | | | |
|---|---|---|---|---|---|---|---|---|
| | | | 1 | | | 2 | | |
| | | | Level 4 | | | | | |
| **Level 3** | **Level 2** | **Level 1** | **1** | **2** | **3** | **1** | **2** | **3** |
| **3** | **2** | **2** | 94 | 94,2 | 103,3 | 97,2 | 97,9 | 92 |
| **3** | **3** | **1** | 94,3 | 99,1 | 103,7 | 95,1 | 93,6 | 93,6 |
| **3** | **3** | **2** | 93,7 | 100,1 | 106,4 | 95,7 | 94,6 | 93,9 |
| **4** | **1** | **1** | 100,9 | 89,1 | 102,4 | 105,2 | 102,1 | 98,2 |
| **4** | **1** | **2** | 102,3 | 88,9 | 101,7 | 104,5 | 103,1 | 98,3 |
| **4** | **2** | **1** | 99,2 | 88,9 | 102,5 | 101,8 | 100,2 | 97,5 |
| **4** | **2** | **2** | 100,3 | 88,9 | 103,6 | 100,7 | 99,8 | 96,2 |
| **4** | **3** | **1** | 101,7 | 94,1 | 103,5 | 97,2 | 100,2 | 104,9 |
| **4** | **3** | **2** | 99,9 | 91,4 | 102,9 | 98,9 | 100,6 | 105,5 |
| | | $m_{3,1}$ | 102,68 | 101,7 | 101,83 | 89,833 | 100,37 | 101,32 |
| | | $m_{3,2}$ | 103,75 | 99,183 | 105,02 | 97,283 | 98,483 | 93,983 |
| | | $m_{3,3}$ | 94,233 | 97,833 | 103,65 | 96,433 | 94,467 | 93,517 |
| | | $m_{3,4}$ | 100,72 | 90,217 | 102,77 | 101,38 | 101 | 100,1 |
| | | $w_{3,j}$ | 18,184 | 24,449 | 1,8346 | 22,875 | 8,6591 | 16,422 |
| | | $m_{4,j}$ | 100,35 | 97,233 | 103,32 | 96,233 | 98,579 | 97,229 |
| | | $w_4$ | 9,2534 | | | 1,3862 | | |

*Calculations are as follows:*

- $m_{3,j} = \sum_1^{n_1 n_2} m_{3,k}/n_3$.
  *For example,* $m_{3,1,1} = (103{,}9 + 101{,}9 + 103{,}7 + 101{,}1 + 102{,}7 + 102{,}8)/6 = 102{,}68$
- $w_{3,j} = Var\left(m_{3,j}\right) = \sum_1^{n_3} \left(m_{3,k} - m_3\right)^2/n_3$.
  *For example,* $w_{3,1,1} = Var(102{,}68; 103{,}75; 94{,}233; 100{,}72) = 18{,}184$
- $w_3 = \sum_1^{n_4 n_5} w_{3,j}{}^2/(n_4.n_5)$.
  *For example,* $w_3 = (18{,}184^2 + 24{,}449^2 + 1{,}8346^2 + 22{,}875^2 + 8{,}6591^2 + 16{,}422^2)/(3 \times 2) = 3{,}8510$
- $m_{4,j} = \sum_1^{n_1 n_2 n_3} x_k/n_1 n_2 n_3$.
  *For example,* $m_{4,1} = (103{,}9 + 101{,}9 + 103{,}7 + 101{,}1 + \cdots + 99{,}2 + 100{,}3 + 101{,}7 + 99{,}9)/24 = 100{,}35$
- $w_{4,j} = Var\left(m_{4,j}\right) = \sum_1^{n_4} \left(m_{4,k} - m_4\right)^2/n_4$.
  *For example,* $w_{4,1} = Var(100{,}35; 97{,}233; 103{,}32) = 9{,}2534$
- $w_4 = Var(m_4) = \sum_1^{n_5} w_{4,j}{}^2/n_5$.
  *For example,* $w_4 = (9{,}2534^2 + 1{,}3862^2)/2 = 5{,}3198$
- $v_4 = 5{,}3198 - 3{,}8510 = 1{,}4688$
- $sd_4 = \sqrt{v_4} = 1{,}2119$

*It shall be noted that the intuitive Equation $v_4 = w_4 - w_3/(n_1.n_2.n_3)$ is wrong and does not provide an estimate without bias of $v_4$ even if, in most cases, the difference between the two is not very large.*

*Same calculations can be conducted to find out that:*

- $v_1 = 1{,}0177$
- $v_2 = 4{,}1425$
- $v_3 = 13{,}854$
- $v_5 = 2{,}5821$

***Example 6:***

*Computation of IC on $v_4$ (estimate of $V_4$) in the case where $n_1 = 2; V_1 = 0{,}1; n_2 = 3; V_2 = 0{,}2; n_3 = 4; V_3 = 0{,}3; n_4 = 5; V_4 = 0{,}4; n_5 = 3; V_5 = 0{,}5$. The results of the subsequent calculations are displayed in Table 6.*

$$SD\left(\frac{v_4}{V_4}\right) = \left(\left(1 + \frac{0{,}3}{4\times 0{,}4} + \frac{0{,}2}{4\times 3\times 0{,}4} + \frac{0{,}1}{4\times 3\times 2\times 0{,}4}\right)^2 \times \frac{2}{(5-1)\times 3} + \left(\frac{0{,}3}{4\times 0{,}4} + \frac{0{,}2}{4\times 3\times 0{,}4} + \frac{0{,}1}{4\times 3\times 2\times 0{,}4}\right)^2 \times \frac{2}{3\times 5\times (4-1)}\right)^{1/2}$$
$$= \left(\frac{(1+0{,}2396)^2}{6} + \frac{2\times 0{,}2396^2}{45}\right)^{1/2} = 0{,}5086$$

*Table 6. Example of calculation of variances of level 4 with 5 nested levels.*

| **α** | **0,025** | **0,05** | **0,1** | **0,2** | **0,5** | **0,8** | **0,9** | **0,95** | **0,975** |
|---|---|---|---|---|---|---|---|---|---|
| $CV_\alpha$ | 1,1831 | 1,1103 | 1,0418 | 0,9814 | 0,9354 | 0,9814 | 1,0418 | 1,1103 | 1,1831 |
| $(v_4/V_4)_\alpha$ **(MCM)** | 0,21±0,02 | 0,29±0,02 | 0,41±0,01 | 0,57±0,01 | 0,94±0,01 | 1,4±0,02 | 1,67±0,02 | 1,92±0,03 | 2,16±0,04 |
| $(v_4/V_4)_\alpha = CV_\alpha + k.SD$ | 0,1864 | 0,2738 | 0,3900 | 0,5533 | 0,9354 | 1,4094 | 1,6935 | 1,9468 | 2,1799 |

# 5 Estimation of a variance with nested levels and unknown ratio between them

## 5.1 Introduction

Because they provide an accurate description of the phenomenon, Equations (3) to (6) are very valuable on the theoretical point of view, but they are of no use in practice because the ratio $V_1/V_2$ is normally unknown when the scope is the determination of an estimate of $V_2$. For the same reason, Equations (8) to (11) also cannot be used in practice in the cases of more than two nested levels.

Moreover, Equation (3) clearly shows that only one equation is available to get an estimate which involves the determination of two values (i.e. $V_1$ and $V_2$).

To try to cope with this issue, we used Equation (3) to produce Equation (12) from which we could derive the Equation (13) by algebraic handling.

$$\frac{n_1.w_2}{v_1} \approx \frac{1+\frac{V_1}{n_1.V_2}}{\frac{V_1}{n_1.V_2}}.F_{(n_2-1,n_2.(n_1-1))} \tag{12}$$

$$\frac{V_1}{n_1.V_2} \approx \frac{1}{\frac{n_1.w_2}{v_1}\times F_{(n_2.(n_1-1),n_2-1)} - 1} \tag{13}$$

We could then hope that the ratio $1/(n_1.w_2/v_1 - 1)$ is an estimator of the key ratio $V_1/(n_1.V_2)$, but it is not a good one, especially when $V_1/(n_1.V_2) > 0{,}1$, i.e. when it would be interesting to use it. Moreover, $1/\left(\frac{n_1.w_2}{v_1}\times\frac{1}{F_{(n_2-1,n_2.(n_1-1))}} - 1\right)$ is not a continuous function (it diverges for an α value for which $F_{(n_2-1,n_2.(n_1-1))} = n_1.w_2/v_1$, centiles of it cannot be computed from the corresponding centiles of the F function. The MCM is needed to determine them. It also follows that a proportion α of the estimates is less than 0, which are wrong because $V_1/(n_1.V_2)$ can never be less than 0.

For all these reasons, Equation (3) alone does not provide an effective solution to determine an IC on $V_2$. To cope with this issue, § 5.2 to 5.4 consider several possibilities that can be implemented to solve this problem, as follows:

- Situations where $V_1$ can be regarded as known;
- Situations where $v_1/n_1 \ll w_2$, for which the influence of the $V_1/(n_1.V_2)$ term is likely to be low;
- Situations where $v_2 < 0$, for which $V_2$ is likely to be low compared to $V_1/n_1$;
- Situations where the results of Equation (1) are unsatisfactory with respect to the intended use of the estimation of $V_2$.

For simplification, each of § 5.2 to 5.4 consider 2 nested levels. Of course, for each of these situations, statements of § 4.3 can be used when more than two nested levels are involved in the estimation process.

## 5.2 Estimation of a variance of nested levels and known variance for level 1

When $V_1$, the variance of level 1, is known, Equation (3) can be simplified into Equation (14) as follows:

$$\frac{v_2}{V_2} \approx \left(1 + \frac{V_1}{n_1.V_2}\right).\frac{\chi^2_{n_2-1}}{n_2-1} - \frac{V_1}{n_1.V_2} \qquad (14)$$

Contrarily to Equation (3), Equation (14) can be easily reversed to get the $V_2/v_2$ ratio, which is the one useful for practice, as follows in Equation (15):

$$\frac{V_2}{v_2} \approx \frac{(n_2-1).\left(1 + \frac{V_1}{n_1.v_2}\right)}{\chi^2_{n_2-1}} - \frac{V_1}{n_1.v_2} \qquad (15)$$

The SD of estimates is then reduced and Equation (4) then becomes Equation (16) as follows:

$$SD\left(\frac{v_2}{V_2}\right) = \left(1 + \frac{V_1}{n_1.V_2}\right)\sqrt{\frac{2}{n_2-1}} \qquad (16)$$

**Conclusion:**

Knowing $V_1$ is a great help to compute an IC on $V_2$ because:

1. An equation is available to compute it exactly;
2. The SD of the distribution of estimates is significantly reduced compared to when $V_1$ is unknown.

## 5.3 Estimation of a variance with 2 nested levels where $v_1/n_1 << w_2$

When $v_1/n_1 \ll w_2$, the influence of the $V_1/(n_1.V_2)$ term is likely to be low, even if it is not impossible that, by chance, the term $\left(1 + \frac{V_1}{n_1.V_2}\right).\frac{\chi^2_{n_2-1}}{n_2-1}$ is in the upper part of its IC and the term $\frac{V_1}{n_1.V_2}.\frac{\chi^2_{n_2.(n_1-1)}}{n_2.(n_1-1)}$ is its lower part of its IC, so that $v_1/(n_1.v_2) \ll V_1/(n_1.V_2)$ and consequently, the estimation of $v_2/V_2$ is of poorer quality than expected.

To check this issue, we used the MCM to generate random $V_1/V_2$ values and observe the resulting $V_2/v_2$.

By the way, using this method and contrarily with Equation (3), we get access to $V_2/v_2$ instead of $v_2/V_2$, which the ratio actually needed in practice. However, the results depend on the distribution of random $v_1/(n_1.v_2)$ values actually input in the calculations. Consequently, care needs to be taken in the choice of this distribution. On our own, we chose a log normal distribution for $V_1/V_2$ with a mean value of 1 and a standard deviation of 1, which produces a distribution with 68% of input values in the interval [0,1;10], 95% in the interval [0,01;100] and 99,7% in the interval [0,001;1000]. This choice enables the calculations to cover the whole field where $V_1/(n_1.V_2) \ll 1 \ll V_1/(n_1.V_2)$, having in mind that situations outside the interval [0,01;100] are 1 – not at all common in practice and 2 – well dealt with by Equation (3) because in those cases, one of the 2 terms of the equation is significantly higher than the other and the handling of it is then highly simplified. We then selected all cases where $v_1/n_1 < 0{,}1.w_2$ (the ratio 0,1 appeared to be an adequate limit to separate cases where $v_1/n_1 \ll w_2$ and the other cases) and checked $v_2/V_2$, ratios as function of $v_2/v_1$. Figure 2 shows an example results of this performance (expressed in SD and not in V), with $n_1 = 2$, $n_2 = 10$ of example 1.

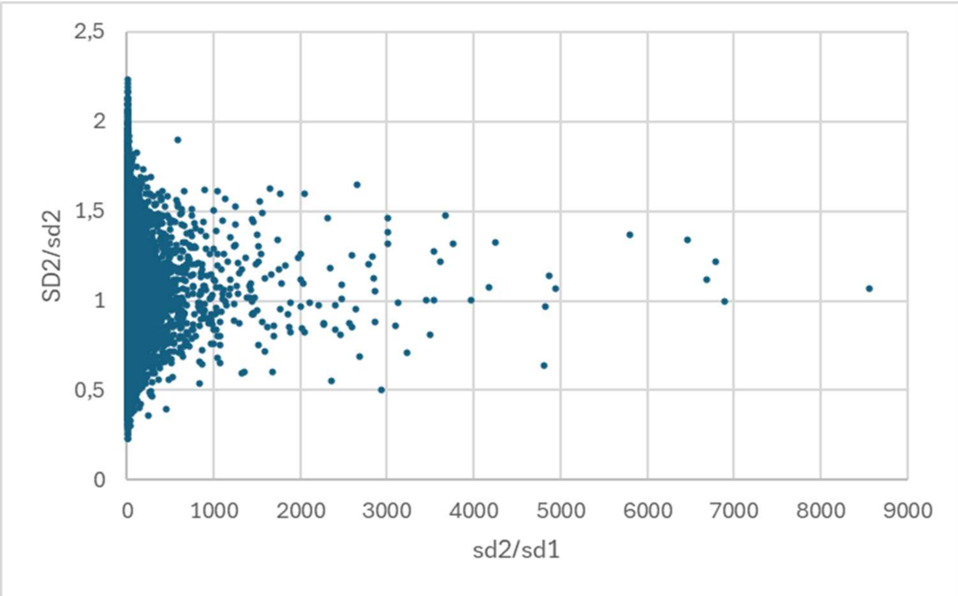


Figure 2: *sd₂/SD₂* ratio as function of *sd₂/sd₁* for situations where $v_1/n_1 < 0{,}1.w_2$.

The results showed that, when $v_1/n_1 < 0{,}1.w_2$, Equation (2) can be used to compute correctly the corresponding IC on $SD_2/sd_2$. However, some very rare occurrences (not shown on the figure for the sake of clarity) can also produce extravagant estimates of $SD_2$ (i.e. very high values for $SD_2/sd_2$, that is to say very strong under estimation of $SD_2$).

## 5.4 Estimation of a variance with 2 nested levels where $v_2 < 0$

We have seen in § 4.2 that Equation (3) happens to produce negative values for $v_2$. We also saw in the example 4 of § 4.4 that there is a threshold value *T* for $n_1.V_2/V_1$ associated with an *α* value for the IC and with the parameters $n_1$, $n_2$, $V_1$ and $V_2$. This means that, when $v_2$ is found negative, an effective upper limit for the IC on $V_2$ may be computed from this threshold value. Even if this computed upper limit is likely to be quite higher than the true value of it, in many cases it provides enough information to solve the practical problem that it is intended to, see example 7 as follows.

***Example 7:***

*In a check of homogeneity of samples as described in ISO 13528 Annex B [3], it is needed to check whether the variance of homogeneity of samples is significantly lower than the expected interlaboratory variance (see example 1). However, in most cases, the variance of repeatability ($V_1$ in the experiment) is often significantly higher than the variance of homogeneity ($V_2$ in the experiment). It then often happens that $v_2 < 0$, with no possibility to get an idea of the IC on it. However, if it appears that $V_2 < T.v_1 \ll V_3$, and the condition for accepting the samples can be regarded as fulfilled even if the exact value of $V_2$ remains completely unknown.*

This $T$ value can be computed by searching 0 values of Equation (3) as function of α, i.e. values of α for which $\left(1+\frac{V_1}{n_1.V_2}\right).\frac{\chi^2_{n_2-1}}{n_2-1}=\frac{V_1}{n_1.V_2}.\frac{\chi^2_{n_2.(n_1-1)}}{n_2.(n_1-1)}$. Handling this equality leads to Equation (17)

$$T \approx \frac{1}{F_{(n_2.(n_1-1),n_2-1)}-1} \tag{17}$$

***Example 8:***

*In a check of homogeneity of samples as described in ISO 13528 Annex B [3], the following results are found:* $w_2=\sum_{j=1}^{10} m_{1j}/10=0{,}216$, $v_1=\sum_{j=1}^{10} v_{1j}/10=3{,}742$, *$n_1$ = 2,* $v_2=0{,}216-3{,}742/2=-1{,}655$, *less than 0.*

*In this case,* $T_{0,95}=1/\left(F_{(n_2.(n_1-1),n_2-1)}-1\right)=1/(3{,}1373-1)=0{,}468$. *On the other hand, the upper limit of IC90($V_1$) (where IC90($V_1$) is the bilateral interval of confidence on* V1*) can be computed as* $MaxV_1=v_1/\chi^2_{n_2.(n_1-1)}=3{,}742/0{,}394=9{,}50$. *We can then conclude that* $V_2<T.MaxV_1/n_1=0{,}468\times 9{,}50/2=2{,}22$ *with a confidence level better than 95%. As it is obvious that* $V_2>0$, *we can conclude that IC90($V_2$) is better than ]0;2,22[.*

This way of computation seems very conservative as it includes 2 steps with a low α value. However, it can be applied only when $v_2<0$, i.e. in cases where $n_1.w_2/v_1<0$. It follows that a covariance applies in corresponding subsequent α values the global $\alpha<\alpha_1.\alpha_2$.

## 5.5 Situations where the results of estimation are unsatisfactory with respect to the intended use of it

When none of the possibilities exposed in § 5.2 to 5.4 provides a satisfactory solution for determining an IC for a nested variance, a new experiment with an increased number *$n_1$* must be considered. Increasing *$n_1$* is the only way to decrease the ratio $V_1/(n_1.V_2)$ which commands the possibility of the determination of it (see upper), because neither *$V_1$* nor *$V_2$* are under the control of the experimenter.

Reducing $V_1/(n_1.V_2)$ to a value less than 0,1 should be the goal to reach, as we saw in § 5.3 that fulfilling such a condition ensures adequate determination of IC.

The problem is then to determine an optimised increase of the *$n_1$* value. This new *$n_1$* value shall be large enough to get an adequate $V_1/(n_1.V_2)$ but it shall also be compatible with technical, economical and practical conditions in which the experiment is conducted. For example, the availability of material or the cost of testing or the amount of time requested to conduct the tests may be a limitation to the increase of the *$n_1$* value. Sometimes, also depending on economical and practical conditions of experimenting, it may be interesting to reduce the *$n_2$* value, so that the total amount of tests $n_1.n_2$ is not much increased by the change of the scheme of experiments.

***Example 9:***

*In a check of homogeneity of samples as described in ISO 13528 Annex B [3], the scheme of experiment may be changed from 10 samples and 2 tests per sample into 3 samples and 7 tests per sample, when this is technically possible (in particular, when it is possible to perform 7 tests on a same sample). The* $V_1/(n_1.V_2)$ *is then increased by 3,5 times.*

In all cases, no general method can determine exactly the new value *$n_1$* that should be chosen because:

1. The ratio $V_1/(n_1.V_2)$ cannot be correctly known in those cases (see Equation (13));
2. And the technical and economical limiting conditions cannot be put in equations.

Consequently, using experience or step-by-step experiments are the best ways to solve this problem.

# 6 Conclusions

Classical equations fail to provide adequate determinations of IC on variances of nested levels. We could find equations that describe well the distributions of variances of nested levels and their scatter, provided that the true values of them is known. Inversing them to express IC on true values of variances as function of their estimations is unfortunately impossible when variances of lower levels are unknown. However, approaching equations can be used when the impact of the variances of lower levels can be expected to be low. Equations to verify this are also proposed.

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