A forgotten fact about the standard deviation

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LETTER TO THE EDITOR

A forgotten fact about the standard deviation

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Dear Sir,

Determination of the Standard Deviation

The calculation of measurement uncertainty should be based on validation data according to established guidelines and standards like the Eurachem/CITAC guide 'Quantifying Uncertainty in Analytical Measurement' 2nd edn [1] or ISO/IEC/EN/DIN 17025(2005) [2]. An important overall method performance parameter is the precision of an analytical (measurement) procedure. The precision is determined as standard deviation. If one looks into a statistical textbook, its calculation seems to be straightforward and without any special issue. In our current work on measurement uncertainty[1] we came across a widely ignored fact about the determination of the standard deviation of measurement results for a small number of measurements.

At the beginning of a project to develop a program for calculating the measurement uncertainty by using the Monte Carlo Method, we generated for the purpose of validating computer code one million random numbers having a normal distribution with a standard deviation of one. If just two samples are drawn from the distribution only 0.7979 is found as mean value of the standard deviation. A first check of the code, which we used to perform the calculations in MatLab[2], did not reveal any error. We repeated the same type of simulations for the standard deviation of three, four and up to ten values. The corresponding script is listed in the appendix of this letter. These simulations with 500,000 values of the standard deviation for just two samplings were repeated 10 times and their results are summarized in Table 1. The mean of the standard deviations approaches relatively fast the expected value of one with increasing sample size. At this stage we started a search for the cause of this observed bias in the internet and found in the German Wikipedia [3] the corresponding explanation and further references.

Reference [4] provides the following explanation for the observed bias in the standard deviation:

Table 1 Results of the simulation to determine the standard deviation of small sampling sizes

Sampling size	Simulation using MatLab		Correction factor - $b(N)$
	Mean std dev (s)	1/mean std dev (s)	
2	0.7982 (6)	1.2529 (9)	1.253314
3	0.8863 (3)	1.1282 (4)	1.128379
4	0.9214 (4)	1.0853 (5)	1.085402
6	0.9515 (3)	1.0510 (4)	1.050936
10	0.9727 (2)	1.0281 (2)	1.028109

The correction factor $b(N)$ is given in Eq. (6). Values in brackets represent one standard deviation for the last digit quoted

[1] Müller M, Wolf M, Gander W, Rösslein M, Measurement Uncertainty Research Group (MURG), ETH (Zürich) and Empa (St Gallen), http://www.mu.ethz.ch

[2] Team MDC MatLab (1994–2006) Natick, MA (USA), The MathWorks

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''Consider the sample standard deviation

$$s \equiv \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_i - \bar{x})^2} \tag{1}$$

for N samples taken from a population with a normal distribution. The distribution of s is then given by

$$f_N(s) = 2\frac{\left(\frac{N}{2\sigma^2}\right)^{(N-1)/2}}{\Gamma\left(\frac{1}{2}(N-1)\right)}\exp\left(-\frac{Ns^2}{2\sigma^2}\right)\cdot s^{N-2} \tag{2}$$

where Γ(z) is a gamma function and

$$\sigma^2 \equiv \frac{Ns^2}{N-1} \quad [5]. \tag{3}$$

Then the mean is given by

$$\langle s \rangle = \sqrt{\frac{2}{N}}\frac{\Gamma\left(\frac{1}{2}N\right)}{\Gamma\left(\frac{1}{2}(N-1)\right)}\sigma \tag{4}$$

$$\langle s \rangle \equiv b(N)\sigma \tag{5}$$

where

$$b(N) \equiv \sqrt{\frac{2}{N}}\frac{\Gamma\left(\frac{N}{2}\right)}{\Gamma\left(\frac{N-1}{2}\right)} \quad [5] \tag{6}$$

The function $b(N)$ is known as c_4 in statistical process control [6] and $s/b(N)$ is an unbiased estimator of σ.''

An extensive survey of the related literature and standards (i.e. ISO 3534 [7], 5725 [8]) revealed that the described fact is widely unknown in the literature and therefore its potentially large effects are ignored. This situation can lead for instance to a significant underestimation of the measurement uncertainty. Let us consider the following example: the repeatability of an analytical result may be taken from a control chart that is based on duplicated measurements. If the repeatability is by far the largest influence quantity, the calculation of the measurement uncertainty results in a value which is about 25% too small. According to our suspicions there might be numerous such effects in other fields.

We have written this letter to bring this very neglected fact to the attention of other colleagues working in quality assurance.

Appendix

MatLab code

```
% Set number of simulations:
sim = 10^6;

% ---------------------------------------
% Generate gaussian random numbers
x = randn(sim,10);

% Initialise target variables
std2 = 0;
std3 = 0;
std4 = 0;
std6 = 0;
std10 = 0;

for i=1:sim
  % Calculate and sum standard deviations of each line with
  % corresponding number of elements
  std2  = std2  + std(x(i,1:2));
  std3  = std3  + std(x(i,1:3));
  std4  = std4  + std(x(i,1:4));
  std6  = std6  + std(x(i,1:6));
  std10 = std10 + std(x(i,1:10));

  % Output progress
  if mod(i, 10000)==0
    i
  end
end

% Finalizing standard deviations, divide by number of lines for
% mean of standard deviations
std2  =  std2/sim
std3  =  std3/sim
std4  =  std4/sim
std6  =  std6/sim
std10 = std10/sim
```

References

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