Ann. Occup. Hyg., pp. 1–5

doi:10.1093/annhyg/men076

Inference on the Symmetric-Range Accuracy

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Received 21 September 2008; in final form 28 October 2008

The symmetric-range accuracy *A* of a sampler is defined as the fractional range, symmetric about the true concentration, that includes a specified proportion of sampler measurements. In this article, we give an explicit expression for *A* assuming that the sampler measurements follow a normal distribution. We propose confidence limits for *A* based on the concept of a 'generalized confidence interval'. A convenient approximation is also provided for computing the confidence limit. Monte Carlo evaluation indicates that the proposed approaches are very satisfactory even for small samples. The statistical procedures are illustrated using an example involving carbon monoxide monitoring.

Keywords: bias; coverage probability; non-central chi-square distribution; normal approximation; tolerance intervals

INTRODUCTION

The development of accuracy criteria is essential for the quantification of measurement accuracy of exposure data. The National Institute of Occupational Safety and Health (NIOSH) accuracy criterion is based on the symmetric-range accuracy A, and the NIOSH accuracy requirement states that a 95% upper confidence limit for A does not exceed 0.25; see NIOSH (1994), especially the chapter by Bartley *et al.* (1994). In general, the symmetric-range accuracy A is defined as the fractional range, symmetric about the true concentration, within which $100\,(1-\alpha)$ % of sampler measurements are to be found. Assuming a normal distribution, Bartley *et al.* (1994) and Bartley (2001) have developed an approximation for A and an approximate 95% upper confidence limit for A. The upper confidence limit is obviously important in order to verify the NIOSH accuracy requirement. The goal of this article is to provide an exact expression for A and an accurate and easy to compute upper confidence limit for A using the generalized confidence interval approach.

If C denotes the true concentration and $\hat{c}$ denotes sampler measurements, the symmetric-range accuracy A satisfies

$$P((1-A)C < \hat{c} < (1+A)C) = 1-\alpha, \qquad (1)$$

where $0<\alpha<1$ and for NIOSH applications $\alpha = 0.05$. Here, we have followed the notations and definitions in Bartley *et al.* (1994) and Bartley (2001). If we assume that $\hat{c}$ follows a normal distribution with mean c and variance σ^2, then we can write

$$\begin{aligned} &P((1-A)C < \hat{c} < (1+A)C) \\ &\quad = P\left(\frac{(1-A)C-c}{\sigma} < \frac{\hat{c}-c}{\sigma} < \frac{(1+A)C-c}{\sigma}\right) \\ &\quad = P\left(\frac{C-c}{\sigma} - \frac{AC}{\sigma} < Z_0 < \frac{C-c}{\sigma} + \frac{AC}{\sigma}\right), \qquad (2) \end{aligned}$$

where $Z_0 = (\hat{c}-c)/\sigma$ is the standard normal random variable. Let $b = (C-c)/\sigma$. Then equation (2) can be expressed as $P(|Z_0 - b| < AC/\sigma)$ or equivalently $P\left((Z_0-b)^2 < A^2C^2/\sigma^2\right)$. Thus, the symmetric accuracy range A should satisfy

$$P\left((Z_0-b)^2 < A^2C^2/\sigma^2\right) = 1-\alpha.$$

Note that $(Z_0-b)^2 \sim \chi^2_1(b^2)$, a non-central chi-square distribution with one degree of freedom and non-centrality parameter b^2. Hence, $A^2C^2/\sigma^2 = \chi^2_{1;1-\alpha}(b^2)$, the $100\,(1-\alpha)$ percentile of the non-central chi-square distribution. Thus,

$$A = \frac{\sigma}{C}\sqrt{\chi^2_{1:1-\alpha}(b^2)}. \qquad (3)$$

In other words, we have an explicit expression for A. It is known that, for a fixed m and $1-\alpha$, the percentile $\chi^2_{m;1-\alpha}(\delta)$ is an increasing function of δ, and

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so the accuracy range A is an increasing function of $|C-c|/\sigma$.

A GENERALIZED CONFIDENCE INTERVAL FOR A

If a sampler is evaluated at known C, then a $100\,\gamma\%$ confidence limit for A can be obtained using the generalized variable approach. This requires the derivation of a generalized pivotal quantity (GPQ) for A. Toward this, let $\hat{c}_1,\ldots,\hat{c}_n$ be sampler measurements, and let $\overline{c}$ and s^2, respectively, denote the mean and variance of the $\hat{c}_i$'s. It is assumed that $\hat{c}_i \sim N(c,\sigma^2)$, where c and σ^2 are the unknown population mean and population variance, respectively. Then,

$$Z=\left(\frac{\sqrt{n}(\overline{c}-c)}{\sigma}\right)\sim N(0,1) \text{ and}$$
$$U^2=\frac{(n-1)s^2}{\sigma^2}\sim \chi^2_{n-1}, \tag{4}$$

where χ^2_{n-1} is a chi-square distribution with $n-1$ degrees of freedom. Furthermore, $\overline{c}$ and s^2 are independently distributed. A GPQ is a function of the random variables $\overline{c}$ and s^2 and the corresponding observed values, say $\overline{c}_{\text{obs}}$ and s^2_{obs}, respectively. A GPQ is required to satisfy two conditions: (i) the distribution of the GPQ should be free of unknown parameters and (ii) if the random variables $\overline{c}$ and s^2 in the definition of the GPQ are replaced by the corresponding observed values $\overline{c}_{\text{obs}}$ and s^2_{obs}, then the GPQ will simplify to the parameter of interest. We shall first illustrate this by constructing GPQs for c and σ, to be denoted by Q_c and Q_σ, respectively. These are given by

$$\begin{aligned} Q_c &= \overline{c}_{\text{obs}} - \frac{\sqrt{n}(c-c)s_{\text{obs}}}{s\quad\sqrt{n}} \\ &= \overline{c}_{\text{obs}} - \frac{\sqrt{n}(c-c)/\sigma s_{\text{obs}}}{s/\sigma\quad\sqrt{n}} \\ &= \overline{c}_{\text{obs}} - \frac{Z}{\sqrt{\frac{U}{n-1}}}\frac{s_{\text{obs}}}{\sqrt{n}} \text{ and } Q_\sigma=\sqrt{\frac{(n-1)s^2_{\text{obs}}}{U^2}}, \end{aligned} \tag{5}$$

where the standard normal random variable Z and the chi-square random variable U^2 are defined in equation (4). It is easy to check that Q_c and Q_σ are GPQs for c and σ, respectively. Further details on constructing GPQs in a similar context can be found in Krishnamoorthy *et al.* (2007); more general results along with other applications can be found in the book by Weerahandi (1995).

A GPQ for a function of c and σ can be obtained by substitution. In particular, a GPQ for $b=|C-c|/\sigma$ is given by $Q_b=|C-Q_c|/Q_\sigma$. Then a GPQ for A is given by

$$Q_A=\frac{Q_\sigma}{C}\sqrt{\chi^2_{1;1-\alpha}(Q_b^2)}. \tag{6}$$

For a given $\overline{c}_{\text{obs}}$ and s^2_{obs}, the distribution of Q_A does not depend on any unknown parameters. Thus, the percentiles of Q_A can be estimated by Monte Carlo simulation. The percentiles so obtained provide confidence limits for A. In particular, the 100 $(1-\alpha)$th percentile of Q_A gives a 100 $(1-\alpha)\%$ upper confidence limit for A. Recall that C is assumed to be known. The algorithm given below can be used to estimate the percentiles of Q_A.

1. For a given sample of measurements $\hat{c}_1,\ldots,\hat{c}_n$, compute the mean $\overline{c}$ and the standard deviation s. Denote the observed values so obtained by $\overline{c}_{\text{obs}}$ and s^2_{obs}.
2. Generate a standard normal random number Z and a χ^2_{n-1}random number.
3. Compute Q_c and Q_b using equation (5) and $Q_b=|C-Q_c|/Q_\sigma$.
4. Using Q_b^2 as the non-centrality parameter, find $\chi^2_{1;1-\alpha}(Q_b^2)$.
5. Compute Q_A in equation (6).
6. Repeat the steps 2–5 a large number of times, say, 10 000.

The 100 $(1-\alpha)$ percentile of the 10 000 Q_A's so generated is a 100 $(1-\alpha)\%$ upper confidence limit for A.

An alternative approximate approach

Notice that to find the percentiles of Q_A, simulation must be carried out a large number of times. For each simulation run, the non-central critical value $\chi^2_{1;1-\alpha}(Q_b^2)$ must be evaluated which makes the calculation more time consuming. To avoid this, we can use the following approximation (see Krishnamoorthy, 2006, p. 212):

$$\chi^2_{m;p}(\delta)\simeq(m+\delta)\left[z_p\sqrt{\left(\frac{2}{9}\right)\frac{m+2\delta}{(m+\delta)^2}} - \left(\frac{2}{9}\right)\frac{m+2\delta}{(m+\delta)^2}+1\right]^3, \tag{7}$$

where z_p is the $100p$th percentile of a standard normal distribution. Specifically, the above approximation with $m=1$, $p=1-\alpha$ and $\delta=Q_{b^2}$ can be used to evaluate $\chi^2_{1;1-\alpha}(Q_b^2)$. If we use the above approximation, then the normal percentile z_p is evaluated only once, and so the simulation of Q_A with the above approximation is less time consuming. Furthermore, as will be seen later in the simulation study section, this approximation is very satisfactory and provides results very close to those based on equation (6).

Remark. If it is assumed that $c=C$, so that $\hat{c}\sim N(C,\sigma^2)$, then $b^2=0$ and the accuracy range A defined in equation (3) becomes $\frac{\sigma}{C}\sqrt{\chi^2_{1;1-\alpha}}$. In this case, the GPQ for A is given by $Q_A=\frac{Q_\sigma}{C}\sqrt{\chi^2_{1;1-\alpha}}$, and the exact $100\gamma\%$ upper confidence limit on the basis of this GPQ is $\left(\frac{(n-1)s^2\chi^2_{1;1-\alpha}}{\chi^2_{n-1;1-\gamma}}\right)^{1/2}$.

CONFIDENCE LIMITS FOR THE TRUE CONCENTRATION

Let A_γ denote the 100 γ% upper confidence limit for A and let $\hat{c}_0$ be a future measurement of C. Then, the interval $\left(\hat{c}_0/(1+A_\gamma), \hat{c}_0/(1-A_\gamma)\right)$ includes C with probability $1-\alpha$. Mathematically,

$$P_{\bar{c},s}\left\{P_{\hat{c}_0}\left((1-A_\gamma)C < \hat{c}_0 < (1+A_\gamma)C \mid \bar{c}, s\right) \geq 1-\alpha\right\} = \gamma,$$

or equivalently

$$P_{\bar{c},s}\left\{P_{\hat{c}_0}\left(\frac{\hat{c}_0}{1+A_\gamma} < C < \frac{\hat{c}_0}{1-A_\gamma} \mid \bar{c}, s\right) \geq 1-\alpha\right\} = \gamma,$$

where $\hat{c}_0 \sim N(c, \sigma^2)$ independently of the sample $\hat{c}_1, \ldots, \hat{c}_n$ that was used to construct the upper confidence limit A_γ.

Suppose the true concentration X for a substance is unknown, $\hat{x}$ be the measurement of X. Further, let us assume that $\hat{x}$ has a normal distribution with mean x and standard deviation σ and the following scaling assumption holds (Bartley, 2001):

$$\frac{x}{c} = \frac{\sigma_x}{\sigma} = \frac{X}{C}.$$

Under this assumption, we have $\frac{x}{\sigma_x} = \frac{c}{\sigma}$ and $\frac{X}{\sigma_x} = \frac{C}{\sigma}$, and using these relations, we obtain

$$\begin{aligned} &P((1-A)X \leq \hat{x} \leq (1+A)X) \\ &= \left(\frac{X-x}{\sigma_x} - \frac{AX}{\sigma_x} < Z_0 < \frac{X-x}{\sigma_c} + \frac{AX}{\sigma_x}\right) \\ &= \left(\frac{C-c}{\sigma} - \frac{AC}{\sigma} < Z_0 < \frac{C-c}{\sigma} + \frac{AC}{\sigma}\right) \\ &= P\left(\left(1-A\right)C \leq \hat{c} \leq \left(1+A\right)C\right). \end{aligned} \quad (8)$$

The above step was obtained using the fact that $\hat{c}$ is distributed as $c + Z_0\sigma$, where Z_0 is a standard normal random variable. Thus, if A_γ is a confidence limit based on the measurements on the reference concentration C and $\hat{x}_1, \hat{x}_2, \ldots$ are a set of measurements on X, then at least a fraction $1-\alpha$ of the intervals

$$\left(\frac{\hat{x}_i}{1+A_\gamma}, \frac{\hat{x}_i}{1-A_\gamma}\right), \quad (9)$$

include X with probability γ.

Finally, note that if $A_{0.95}$ is <0.25, then we conclude that the measuring method satisfies the NIOSH requirement.

SIMULATION STUDIES

To appraise the validity of the above generalized confidence intervals for A, we estimated the coverage probabilities of the 95% upper confidence limits for A based on the GPQ equation (6) and the approximation equation (7). As the family of normal distributions is location–scale invariant and the accuracy range is also location–scale invariant, without loss of generality, we can choose $C = 1$ and $\sigma = 1$. For evaluating coverage probabilities of the confidence limits. We estimated the coverage probabilities for the sample sizes $n = 10, 20, 30, \ldots$ and 50 and for a nominal confidence level of 0.95. The estimated coverage probabilities are given in Table 1. For a good estimation procedure, the estimated coverage probabilities should be close to the nominal level 0.95. We first observe from Table 1 that the coverage probabilities of the generalized confidence limits and those of the approximation are practically the same. Furthermore, the coverage probabilities are very close to the nominal confidence level 0.95, except for the cases where the values of c are close to C and n is small; in these cases, the confidence limits are slightly conservative. In general, the generalized confidence interval approach and the approximation procedure seem to work very well.

AN EXAMPLE

We shall use the gas monitor data described in Shulman and Smith (2002) to illustrate the methods of this article. These data represent measurements of carbon monoxide at several known concentrations, made by various monitors. More details on the collection of measurements and calibration of monitors, etc. can be found in the above article. We shall use

Table 1. Coverage probabilities of 95% upper confidence limits for A based on the GPQ equation (6) and based on the approximation equation (7) for $C = 1$ and $\sigma = 1$; the coverage probabilities corresponding to the approximation are given in parentheses

	c					
n	1	1.4	1.8	3	4	5
10	0.97 (0.97)	0.96 (0.96)	0.95 (.94)	0.95 (0.95)	0.95 (0.95)	0.95 (0.95)
20	0.96 (0.96)	0.96 (0.95)	0.95 (0.94)	0.95 (0.95)	0.95 (0.95)	0.95 (0.95)
30	0.96 (0.96)	0.95 (0.94)	0.95 (0.95)	0.95 (0.95)	0.95 (0.95)	0.95 (0.95)
50	0.95 (0.95)	0.95 (0.95)	0.95 (0.95)	0.95 (0.95)	0.95 (0.95)	0.95 (0.95)

the set of 12 measurements by the monitor E at the concentration of 238.1 for setting a 95% upper confidence limit for the symmetric-range accuracy A and another set of 12 measurements by the same monitor at the concentration of 102 for setting prediction intervals. That is, for the sake of illustration, we regard $C = 238.1$ as the reference concentration and the monitor responses as $\hat{c}_1, \ldots, \hat{c}_{12}$. We shall denote the measurements at the concentration $X = 102$ as $\hat{x}_1, \ldots, \hat{x}_{12}$. The monitor responses are given in Table 2 when $C = 238.1$ and $X = 102$. Normal probability plots of both sets of measurements in Fig. 1 clearly show that the normality assumption for both data sets is tenable.

The mean and standard deviation of the measurements at the concentration $C = 238.1$ are $\overline{c} = 215.03$ and $s = 7.3304$, respectively. The 95% upper confidence limit for the accuracy range A on the basis of the generalized confidence interval approach with 10 000 simulation runs is $A_{0.95} = 0.1829$. That is, for 95% of such sampler evaluations, at least a fraction 0.95 of intervals of the form $\left(\frac{\hat{c}}{1+0.1829}, \frac{\hat{c}}{1-0.1829}\right)$ would include the true concentration. We also computed the 95% upper confidence limit using the approximation

Table 2. Monitor measurements of carbon monoxide

Measurements $\hat{c}$ at the true concentration $C =$	238.1, 220.3, 225.0, 217.0, 210.0, 202.0, 210.0, 202.0, 205.0, 225.0, 220.0, 215.0, 217.0, 209.0
Measurements $\hat{x}$ at the true concentration $X =$	102, 100.2, 99.5, 94.0, 91.7, 88.9, 88.0, 97.4, 98.5, 96.0, 96.2, 96.3, 94.3

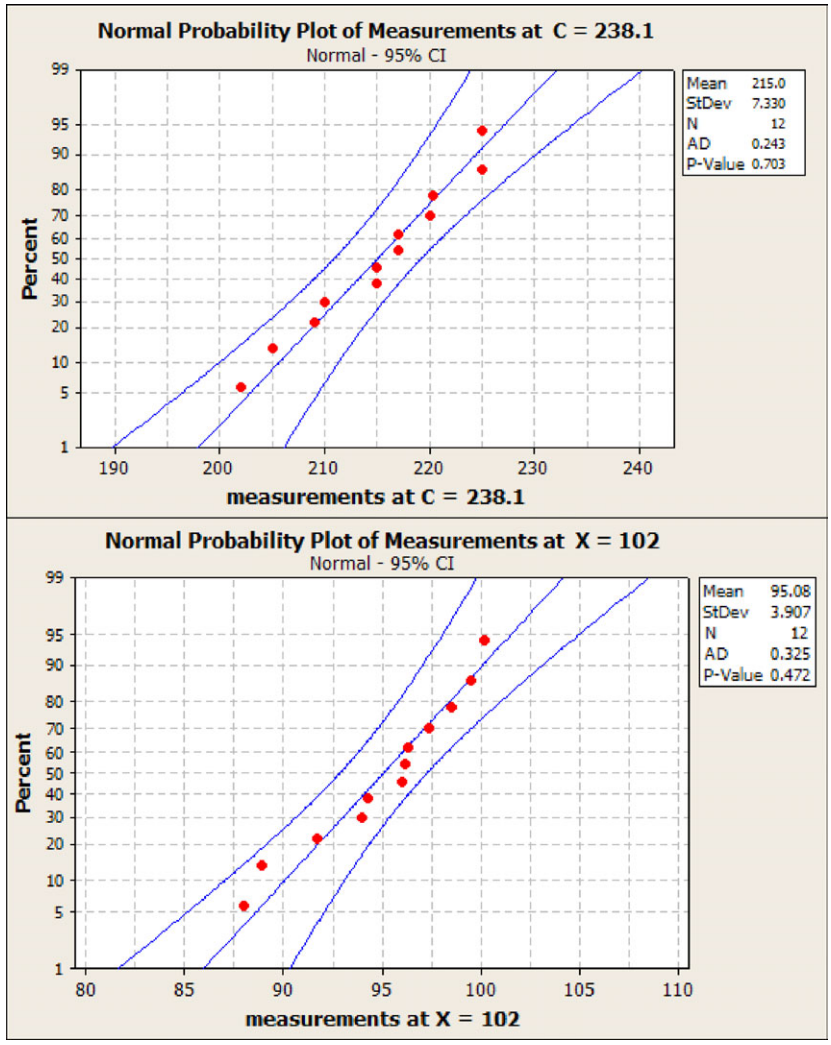

Fig. 1. Normal probability plots of monitor measurements.

equation (7) as $A_{0.95} = 0.1823$. Notice that this is very close to the confidence limit 0.1829, which is based on equation (6).

To illustrate Bartley's (2001) approach, let us define the bias Δ and true relative standard deviation (TRSD) by

$$\Delta = \frac{c - C}{C} \quad \text{and} \quad \text{TRSD} = \frac{\sigma}{C}.$$

Replacing c by $\bar{c} = 215.03$ and σ by $s = 7.3304$, we get estimates $\hat{\Delta} = 0.0965$ and $\widehat{\text{TRSD}} = 0.0308$. As the bias magnitude is evidently large relative to TRSD, the accuracy range A is closely approximated by

$$A = -\Delta + 1.645 \times \text{TRSD}. \qquad (10)$$

The 95% upper confidence limit for this approximation is given by

$$A_{0.95} = -\hat{\Delta} - \frac{\widehat{\text{TRSD}}}{\sqrt{n}}\, t_{n-1;.05}(\delta), \qquad (11)$$

where $t_{n-1;.05}(\delta)$ is the fifth percentile of a non-central t distribution with degrees of freedom $n - 1$ and non-centrality parameter $\delta = -1.645\sqrt{n} = -1.645\sqrt{12} = -5.698$. Noting that $n = 12$ and $t_{11;.05}(-5.698) = -9.479$, we see that equation (11) results in $A_{0.95} = 0.181$. Notice that Bartley's approximate procedure also produced the upper confidence limit that is very close to those based on our methods given in the preceding paragraph.

Thus, agreement is apparent between the generalized variable approach and Bartley's approach based on classical pivots, in this specific case. In more complex yet practical situations, the generalized confidence limit may provide a solution, when classical pivots are unavailable. As an example, suppose a sampling method using a variable sampler is evaluated. In this case, inter-sampler variation exists, independently of the intra-sampler variability. Although equation (10) remains accurate, the confidence limit in equation (11) is no longer valid if the inter-sampler variation is significant. However, the generalized confidence limit procedure still applies, as has been noted in Krishnamoorthy *et al.* (2007) for a different class of problems.

The prediction intervals for $X = 102$ are constructed using the formula in equation (9), and these intervals along with the measurements $\hat{x}$ are given in Table 3. We observe that all the intervals contain the true concentration of 102.

Table 3. Prediction intervals for the true concentration

$\hat{x}$	$\hat{x}/(1 + A_{0.95})$	$\hat{x}/(1 - A_{0.95})$
100.2	84.707	122.629
99.5	84.115	121.772
94.0	79.466	115.041
91.7	77.521	112.226
88.9	75.154	108.799
88.0	74.393	107.698
97.4	82.340	119.202
98.5	83.270	120.548
96.0	81.156	117.489
96.2	81.326	117.733
96.3	81.410	117.856
94.3	79.719	115.408

DISCUSSION

The generalized variable approach has earlier been used to address several problems relevant to the analysis of occupational exposure data; see Krishnamoorthy and Mathew (2002) and Krishnamoorthy *et al.* (2006, 2007). In the present article, we provide yet another application: the computation of confidence limits for the symmetric-range accuracy. Numerical results show that the resulting confidence limits exhibit satisfactory performance in terms of providing coverage probabilities close to the nominal level, even for small sample sizes. Since reliable criteria for the quantification of measurement accuracy is crucial in industrial hygiene applications, it is hoped that the proposed methodology will be relevant and useful in such applications.

Acknowledgements—The authors are thankful to Stanley Shulman for bringing the symmetric-range accuracy problem to their attention and for providing the gas monitor data. They are grateful to David Bartley for providing useful comments and suggestions and for his observations concerning the agreement between the generalized variable approach and his approach.

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