IOP Publishing Metrologia

Metrologia 46 (2009) 81-86

doi:10.1088/0026-1394/46/1/010

Fiducial intervals for the magnitude of a complex-valued quantity

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Received 26 August 2008, in final form 15 October 2008 Published 19 December 2008 Online at stacks.iop.org/Met/46/81

Abstract

This paper discusses a fiducial approach for constructing uncertainty intervals for the distance between k normal means and the origin. When k=2 this distance is equivalent to the magnitude of a complex-valued quantity. A simulation study was conducted to assess the frequentist performance of the proposed fiducial intervals and to compare their performance with the methods from the *Guide to the Expression of Uncertainty in Measurement* and from Supplement 1 to the 'Guide to the Expression of Uncertainty in Measurement'—Propagation of Distributions using a Monte Carlo Method. Our results indicate that the fiducial intervals generally outperform the GUM and GUM Supplement 1 methods with respect to frequentist coverage probabilities. Computer programs for calculating the fiducial intervals, written using open-source software, are listed.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The recent draft of Supplement 1 [1] to the *Guide to the Expression of Uncertainty in Measurement* (GUM) has generated much interest within the metrology community. Supplement 1 is intended to provide an alternative method to the GUM approach for propagation of uncertainties when the GUM method does not lead to satisfactory approximations. Many authors have written papers on both methodology and applications related to Supplement 1 in measurement journals. For example, see the papers, and cited references listed therein, in a special issue, volume 43(4), of *Metrologia*.

In a typical measurement equation, the measurand is modelled as a function of one or more input quantities. Based on the measurement equation, the Supplement 1 method obtains a probability density function (pdf) for the measurand by propagating the pdfs of the input quantities. The resulting pdf describes one's knowledge of the measurand given the observed data and assumptions made in assigning the joint pdf of the input quantities used in propagation. Since the joint probability distribution for the input quantities is generally an approximation, and since the measurement equation itself is an idealization of reality, the derived pdf for the measurand should be interpreted as approximate as well.

In many standard situations, the pdf for the measurand obtained using the Supplement 1 method is identical to the *posterior* distribution for the measurand of a Bayesian analysis with non-informative improper priors [2]. Strictly speaking, however, the method of Supplement 1 is not equivalent to the standard Bayesian approach based on the use of Bayes Theorem. This standard Bayesian approach, unlike the Supplement 1 method, requires the specification of prior distributions for all parameters in the measurement equation, including the measurand, see [3] for an example.

Another approach that associates a distribution with a measurand is fiducial inference. In this approach, a probability distribution, called the fiducial distribution, for the measurand conditional on the data is obtained based on the *structural equation* that relates the measurements to model parameters and error processes whose distributions are fully known. Statistical procedures based on fiducial inference have been developed for various applications in metrology, for example, see [4–8].

The Supplement 1 and fiducial methods will produce different results in general. However, for measurements assumed to be from univariate normal distributions, many uncertainty intervals obtained using these two methods are very similar, if not identical. For example, in the case of a random sample from a normal distribution with mean μ and variance σ^2 ($N(\mu, \sigma^2)$), the uncertainty intervals for μ calculated by both methods are the same. Both intervals are derived from the same probability distribution for μ , which is a scaled and shifted t distribution.

Although neither the Supplement 1 method nor the fiducial method is based on a frequentist view of inference, it is of interest to examine the 'long-run success rate' or the frequentist coverage of the uncertainty intervals produced by these methods. Hannig *et al* [9] showed that the fiducial intervals have correct asymptotic frequentist coverage under certain conditions that are almost always met in practical applications. Many simulation studies reported in the literature also appear to support the claim that coverage probability of fiducial intervals for various applications are sufficiently close to their stated value. This frequentist property also holds for those of the Supplement 1 intervals that are equivalent to the corresponding fiducial intervals.

Hannig *et al* [9] discussed an example where the conditions for correct asymptotic frequentist coverage of a straightforward fiducial interval are not met. The example is as follows. Suppose X_{i1}, \ldots, X_{in} are random samples from $N(\mu_i, \sigma^2)$, $i = 1, \ldots, k$. Let

$$\theta^2 = \sum_{i=1}^k \mu_i^2. \tag{1}$$

Then the fiducial intervals for θ based on the scaled and shifted t probability distributions of μ_i have unsatisfactory frequentist performance when θ is small compared with σ . the Supplement 1 interval is identical to the straightforward fiducial interval for θ in this example, it also suffers the poor frequentist performance when θ is small. Hall [10] used a simpler version (k = 2 and known σ) of this example to demonstrate the poor frequentist performance of the Supplement 1 intervals and questioned the widely held view that the Supplement 1 method should be used to validate the GUM method. Hannig et al [9] also proposed a fiducial interval for θ that does not suffer poor frequentist performance when θ is small. This fiducial interval is based on a new set of structural equations, which is different from the usual one based on the scaled and shifted t distributions. In this paper we discuss the development of this fiducial interval for θ in detail.

The rest of the paper is organized as follows. Section 2 briefly reviews the uncertainty intervals for θ based on the scaled and shifted t density function of each μ_i and points out why these intervals have poor frequentist performance when θ is small. In section 3 we go through the detailed derivation of an alternative fiducial interval for θ and outline a procedure for calculating the interval. Section 4 describes a simulation study, similar to the one given by Hall [10], to examine the long-run success rate of the uncertainty intervals for θ . We conclude with some summary remarks in section 5.

2. Straightforward fiducial/Supplement 1 intervals

Let

$$\bar{X}_i = \frac{1}{n} \sum_{i=1}^n X_{ij}$$
 (2)

and

$$S_w^2 = \frac{1}{k(n-1)} \sum_{i=1}^k \sum_{j=1}^n (X_{ij} - \bar{X}_i)^2.$$
 (3)

Then \bar{X}_i is normally distributed with mean μ_i and variance σ^2/n , we write $\bar{X}_i \sim N(\mu_i, \sigma^2/n)$. Also, $k(n-1)S_w^2/\sigma^2 \sim \chi^2(k(n-1))$. We use $\chi^2(v)$ to denote the χ^2 distribution with v degrees of freedom. With these distributional properties, we can write

$$\bar{X}_i = \mu_i + \frac{\sigma}{\sqrt{n}} Z_i, \qquad i = 1, \dots, k$$

$$S_w^2 = \frac{\sigma^2 W}{k(n-1)},$$
(4)

where Z_i , $i=1,\ldots,k$, are independent standard normal random deviates and $W\sim \chi^2(k(n-1))$. By solving the above structural equations, a fiducial quantity (FQ) for μ_i can be obtained as

$$\tilde{\mu}_i = \bar{x}_i - \frac{s_w}{\sqrt{n}} T_i,$$

where \bar{x}_i and s_w are the realized values of \bar{X}_i and S_w , respectively, and $T_i \sim t(k(n-1))$, a t distribution with k(n-1) degrees of freedom. The fiducial distribution of μ_i , which is the distribution of $\tilde{\mu}_i$, is a scaled and shifted t distribution. An FQ for θ is then given by

$$\tilde{\theta} = \sqrt{\sum_{i=1}^{k} \left(\bar{x}_i - \frac{s_w}{\sqrt{n}} T_i\right)^2}.$$
 (5)

The FQ in (5) enables us to generate realizations from the fiducial distribution of θ . Once the realizations are obtained, we can use them to construct the fiducial interval for θ . For example, an equal tail, 95% fiducial interval for θ is given by $(\tilde{\theta}_{0.025}, \ \tilde{\theta}_{0.975})$, where $\tilde{\theta}_{\beta}$ is the β quantile of the realizations. The uncertainty intervals for θ based on the Supplement 1 method are identical to the fiducial intervals based on the FQ in (5).

In (5), T_i takes, at random, a range of positive and negative values. However, the realizations generated based on (5) are always positive. Consequently, the lower bound of the fiducial interval for θ will be positive and hence may not cover θ when θ is close to 0. This explains the poor frequentist performance of the intervals when θ is small.

3. Alternative fiducial intervals

To develop an alternative fiducial interval for θ that does not suffer poor frequentist performance, we need to utilize some results from a *non-central* χ^2 distribution. If Z_1, \ldots, Z_k are independent standard normal random variables then the

distribution of $\sum_{i=1}^{k} Z_i^2$ is a χ^2 with k degrees of freedom. If δ_i , $i=1,\ldots,k$, are constants, then the distribution of

$$\sum_{i=1}^{k} (Z_i + \delta_i)^2$$

is called a non-central χ^2 with k degrees of freedom and the non-centrality parameter $\lambda = \sum_{i=1}^k \delta_i^2$ [11, p 130]. We use the symbol $\chi^2(k,\lambda)$ to denote this non-central χ^2 distribution. Note that $\chi^2(k)$ is equivalent to $\chi^2(k,0)$.

Let

$$S_h^2 = \sum_{i=1}^k \bar{X}_i^2 = \sum_{i=1}^k \left(\mu_i + \frac{\sigma}{\sqrt{n}} Z_i \right)^2, \tag{6}$$

where $Z_1, ..., Z_k$ are independent standard normal random variables. We observe that S_h^2 is independent of S_w^2 defined in (3), and

$$\frac{nS_h^2}{\sigma^2} = \sum_{i=1}^k \left(\frac{\sqrt{n}\mu_i}{\sigma} + Z_i\right)^2 \sim \chi^2(k,\lambda),$$

with the non-centrality parameter

$$\lambda = \sum_{i=1}^{k} \left(\frac{\sqrt{n}\mu_i}{\sigma} \right)^2 = \frac{n\theta^2}{\sigma^2},$$

where θ is given in (1). Since the parameter of interest θ appears in the non-centrality parameter of the distribution of S_h^2 , we need to develop a structural equation that relates S_h^2 to λ .

Let $X \sim \chi^2(k, \lambda)$ and

$$F_{k}(x,\lambda) = P(X \leq x).$$

That is, $F_k(x, \lambda)$ is the cumulative distribution function of $\chi^2(k, \lambda)$. If $F_k(x, \lambda) = u$, $0 \le u \le 1$, we define two inverse functions of $F_k(x, \lambda)$. The first one is $F_k^{-1}(u, \lambda) = x$ when $F_k(x, \lambda)$ is viewed as a function of x (with λ fixed). The second one is $G_k(u, x) = \lambda$ when $F_k(x, \lambda)$ is viewed as a function of λ (with x fixed). Let

$$U = F_k \left(\frac{nS_h^2}{\sigma^2}, \frac{n\theta^2}{\sigma^2} \right). \tag{7}$$

Then

$$P[U \leqslant u] = P\left[F_k\left(\frac{nS_h^2}{\sigma^2}, \frac{n\theta^2}{\sigma^2}\right) \leqslant u\right]$$

$$= P\left[\frac{nS_h^2}{\sigma^2} \leqslant F_k^{-1}\left(u, \frac{n\theta^2}{\sigma^2}\right)\right]$$

$$= F_k\left(F_k^{-1}\left(u, \frac{n\theta^2}{\sigma^2}\right), \frac{n\theta^2}{\sigma^2}\right)$$

$$= u.$$

That is, U is a uniform random variable over the interval (0, 1). The above result is generally known as *probability* integral transform [12, p 202], which states that if X is a random variable with continuous cumulative distribution function $F_X(x)$, then $U = F_X(X)$ is a uniform random

variable over the interval (0, 1). For the above application, $X = nS_h^2/\sigma^2$.

From (7), by using the definition of the second inverse of $F_k(x, \lambda)$, we have

$$\frac{n\theta^2}{\sigma^2} = G_k \left(U, \frac{nS_h^2}{\sigma^2} \right). \tag{8}$$

This relates the model parameters (θ, σ) to observable statistic S_h and U whose distribution (uniform) is fully known. Together with the structural equation for σ^2 in (4), i.e.

$$\sigma^2 = \frac{S_w^2}{W/[k(n-1)]}$$

we obtain the following FQ for θ

$$\tilde{\theta}^* = \frac{\tilde{\sigma}}{\sqrt{n}} \sqrt{G_k \left(U, \frac{ns_h^2}{\tilde{\sigma}^2} \right)} = \frac{s_w}{\sqrt{nW/[k(n-1)]}} \times \sqrt{G_k \left(U, \frac{ns_h^2}{s_w^2/(W/[k(n-1)])} \right)}. \tag{9}$$

A single realization of $\tilde{\theta}^*$ may be generated as follows.

- 1. Generate $U_0 \sim \text{uniform}(0, 1)$ and $W_0 \sim \chi^2(k(n-1))$.
- 2. Evaluate

$$\lambda_0 = G_k \left(U_0, \frac{ns_h^2}{s_n^2/(W_0/[k(n-1)])} \right),$$

which is equivalent to obtaining λ_0 such that

$$F_k\left(\frac{ns_h^2}{s_w^2/(W_0/[k(n-1)])}, \, \lambda_0\right) = U_0. \tag{10}$$

The existence of a single solution λ_0 is guaranteed since $F_k(x, \lambda)$ is a decreasing function of λ . Also if

$$F_k\left(\frac{ns_h^2}{s_w^2/(W_0/[k(n-1)])}, 0\right) \leqslant U_0$$

then $\lambda_0 = 0$ by definition. See figure 1 for an illustration.

3. Calculate

$$\tilde{\theta}^* = \frac{s_w \sqrt{\lambda_0}}{\sqrt{nW_0/[k(n-1)]}}.$$

A program for generating realizations of $\tilde{\theta}^*$, based on R software [13], is listed in the appendix.

Note that $\tilde{\theta}^*$ can have zero as its realization since λ_0 can be zero. The smaller the value of s_h is, the more likely it is that

$$F_k\left(\frac{ns_h^2}{s_n^2/(W/[k(n-1)])}, 0\right) \leqslant U$$

and hence $\lambda_0 = 0$. We use the example in [10] to illustrate the difference between the fiducial distributions based on FQs in (5) and (9). In this example, the measurand is the magnitude of a complex-valued quantity:

$$\Gamma = \Gamma_1 + i\Gamma_2.$$

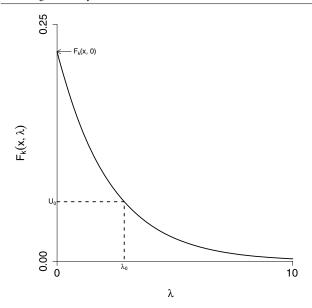


Figure 1. A plot of $F_k(x, \lambda)$ as a function of λ with x fixed. The maximum of $F_k(x, \lambda)$ is $F_k(x, 0)$. If $U_0 \ge F_k(x, 0)$ then $\lambda_0 = 0$. If $U_0 < F_k(x, 0)$ a solution λ_0 is found such that $F_k(x, \lambda_0) = U_0$.

That is, the measurand is

$$|\mathbf{\Gamma}| = \sqrt{\Gamma_1^2 + \Gamma_2^2}.$$

Also, measurements X_1 and X_2 , which estimate Γ_1 and Γ_2 , respectively, are available. In addition, we assume $X_1 \sim N(\Gamma_1, \sigma^2/n)$ and $X_2 \sim N(\Gamma_2, \sigma^2/n)$ with known σ . Comparing this example with the general case discussed above, we have k=2. Suppose $\sigma/\sqrt{n}=1$ and $x_1^2+x_2^2=0.3$ (arbitrary units). Figure 2 displays the fiducial density functions of $|\Gamma|$; the dashed line is the density function using 10 000 realizations generated from the FQ in (5), and the solid line is based on the FQ in (9). Both density functions are computed using the kernel density estimation method [14]. Some statistics for both densities are listed in table 1. These two density functions are very different when $x_1^2+x_2^2$ is small.

Next, suppose $\sigma/\sqrt{n}=1$ and $x_1^2+x_2^2=20$ (arbitrary units). Figure 3 displays the fiducial density functions of $|\Gamma|$ based on the FQs in (5) and (9). In this case, they are more similar. The equal tails, 95% fiducial intervals for $|\Gamma|$ are (2.685, 6.584) and (2.377, 6.345) based on densities 1 (dashed line) and 2 (solid line), respectively.

4. Performance evaluation

We conduct a simulation study to evaluate the frequentist performance of the uncertainty intervals for θ discussed above. We also include the GUM intervals (see [10]) in the study. For given k and n, it can be shown that the coverage probabilities of the intervals for θ depend only on θ/σ . We only consider k=2 here results for other values of k are similar. Three values of n are used: 1, 5 and 20. When n=1, the degrees of freedom for S_w^2 is 0, we assume σ is known in this case as in the

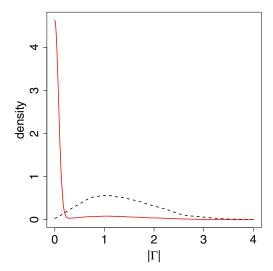


Figure 2. Density functions for $|\Gamma|$ when $\sigma/\sqrt{n}=1$ and $x_1^2+x_2^2=0.3$ using the Supplement 1 (dashed line) and the fiducial (solid line) methods.

Table 1. Statistics for two density functions in figure 2.

Density	Mean	St. dev.	2.5% Tile	97.5% Tile
Dashed	1.358	0.706	0.244	2.958
Solid	0.182	0.521	0.000	1.961

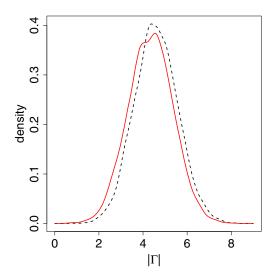


Figure 3. Density functions for $|\Gamma|$ when $\sigma/\sqrt{n}=1$ and $x_1^2+x_2^2=20$ using the Supplement 1 (dashed line) and the fiducial (solid line) methods.

simulation reported by Hall [10]. Values of θ/σ used are 0.1, 0.2, 0.5, 1, 2 and 5. Table 2 displays the number of successes out of 1000 for the nominally 95% GUM, Supplement 1, and fiducial intervals on θ for various combinations of n and θ/σ . It also displays the mean values of the estimates of θ/σ . The estimates of θ/σ are the midpoint of the GUM interval and the means of the Supplement 1 and fiducial density functions of θ/σ . Both the Supplement 1 and fiducial procedures are based on 10 000 Monte Carlo samples.

Table 2. The number of successes (a) out of 1000 for uncertainty intervals on θ , and the mean value (b) of the estimate of θ/σ based on the GUM, Supplement 1, and fiducial procedures when k=2.

n	θ/σ	GUM	Sup. 1	Fiducial
1	0.1	881ª	0	946
		1.27^{b}	1.78	0.90
	0.2	909	0	954
		1.26	1.77	0.89
	0.5	937	771	945
		1.32	1.82	0.96
	1.0	955	917	955
		1.54	1.98	1.19
	2.0	967	950	949
		2.29	2.57	2.01
	5.0	942	941	938
		5.13	5.23	5.02
5	0.1	853	114	951
		0.56	0.84	0.40
	0.2	876	659	952
		0.58	0.85	0.42
	0.5	895	895	935
		0.74	0.96	0.58
	1.0	904	938	947
		1.11	1.26	0.97
	2.0	895	949	943
		2.04	2.11	1.96
	5.0	894	946	949
		5.01	5.04	4.99
20	0.1	912	683	957
		0.30	0.41	0.22
	0.2	925	880	936
		0.34	0.44	0.26
	0.5	949	958	950
		0.55	0.61	0.48
	1.0	941	961	953
		1.02	1.05	0.99
	2.0	924	945	947
		2.02	2.03	2.01
	5.0	917	946	944
		5.00	5.01	5.00

Table 2 indicates that the Supplement 1 intervals have insufficient frequentist coverage when θ/σ is small. The GUM intervals also have insufficient frequentist coverage in most cases. One could argue that θ/σ , the signal-to-noise ratio, would not be small in most metrological applications, and we believe that is a valid point. However, for few cases where θ/σ is small, the fiducial procedure can be recommended for constructing uncertainty intervals for θ .

The mean value of the estimate of θ/σ reveals that when θ/σ is small, both the Supplement 1 and fiducial density functions of θ/σ are highly skewed. As θ/σ increases, the density functions become more symmetric and are centred around the nominal value of θ/σ .

5. Conclusion

In this paper we have discussed a fiducial solution for constructing the uncertainty interval on $\sqrt{\mu_1^2 + \cdots + \mu_k^2}$, where μ_i are the means of the k normal distributions with common variance σ^2 . This fiducial interval maintains the nominal

frequentist coverage in all situations, while the Supplement 1 interval suffers poor frequentist performance when all of the μ_i are small relative to their corresponding σ_i . This issue could be mitigated by appropriately increasing the number n of repeat measurements of the input quantities in the measurement equation since $\sigma_i = \sigma/\sqrt{n}$ where σ is the standard deviation associated with individual measurements. However this is not always possible due to cost constraints. What is noteworthy is the fact that, when the signal-to-noise ratio is low and for a given level of resources, the fiducial approach gives tighter uncertainty intervals while maintaining the coverage rate close to the advertised value.

In conclusion, while the Supplement 1 method performs adequately in many instances, it can have difficulties maintaining the claimed coverage rates, especially when the measurand is not a one-to-one function of the input quantities, such as $\theta = \sqrt{\sum_{i=1}^k \mu_i^2}$. In such cases, the frequentist performance of the Supplement 1 intervals should be examined and alternative procedures may be considered.

Appendix

We list an R function fnc that generates realizations from the fiducial distribution of θ based on the FQ in (9).

```
fnc = function(SH, SW, k, n, dfW=k*(n-1),
               nrun=10000) {
 # generate realizations from the
 # distribution of FQ in (9)
 if (dfW <= 0) Wx = rep(SW, nrun)
 else Wx = SW/(rchisq(nrun, dfW)/dfW)
 Vx = n*SH/Wx
 Ux = runif(nrun)
 Zmat = cbind(Ux, Vx)
 qout = apply(Zmat, 1, lambda, k=k)
 qout = sqrt(qout*Wx/n)
 qout
lambda = function(uin, k) {
 if (pchisq(uin[2], k) \le uin[1]) out = 0
 else {
   out = NA
   if ((pchisq(uin[2], k) - uin[1])*
      (pchisq(uin[2], k, maxpt) -
       uin[1]) < 0) {
       tmp = uniroot(function(arg, xin, k)
             pchisq(xin[2], k, arg) -
               xin[1], c(0, 1400),
               tol=0.0001, xin=uin, k=k)
       out = tmp$root
  }
 }
 out
```

The function fnc has six mandatory and optional arguments:

- 1. Value of $\sum_{i=1}^k \bar{x}_i^2$. 2. Value of $\sum_{i=1}^k \sum_{j=1}^n (x_{ij} \bar{x}_i)^2/(k(n-1))$. 3. Number of groups.
- 4. Number of observations within each group.
- 5. Degrees of freedom for S_w^2 and the default value is k(n-1). Use a non-positive number for infinity.
- 6. Number of fiducial samples desired. The default is 10 000.

The function also calls another function lambda to solve for λ_0 in equation (10). The output contains the desired number of samples from the fiducial distribution of θ . With this function, the following commands may be used to generate 10000 realizations for the example in section 3 with $x_1^2 + x_2^2 = 0.3$ and $\sigma = 1$:

$$> fs = fnc(0.3, 1, 2, 1)$$

and calculate a 95% fiducial interval for $|\Gamma|$

Acknowledgments

The authors are grateful to the referees for their valuable suggestions. This work is a contribution of the National Institute of Standards and Technology and is not subject to copyright in the United States.

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