Subjective fiducial inference for the Grubbs model

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1 Introduction

Several areas of knowledge, such as medicine, physics, engineering, agronomy, economics, biology, social sciences, among others, have shown interest in the problem of methods comparison studies. For that, the Grubbs (1983) model can be considered, which is often used to assess the relative agreement between two or more analytical instruments designed to measure a same quantity of interest.

Consider two instruments for measuring a quantity of interest x and a set of readings of experimental units. Thus, let x_i be the unobservable measurement, while X_i and Y_i are the measured values obtained by the instruments I_1 and I_2, respectively, in i-th unit. Relating these variables, we have

$$Y_i = \beta_0 + x_i + \varepsilon_i \quad \text{and} \quad X_i = x_i + u_i, \quad i = 1, \ldots, n, \tag{1}$$

where β_0 is the bias or systematic error of the instrument I_2 with respect to the instrument I_1. Assume in (1) that x_i are independent and distributed as a normal random variable with mean μ_x and variance σ_x^2, denoted by $\mathcal{N}(\mu_x, \sigma_x^2)$. Moreover, assume ε_i and u_i are independent random errors following $\mathcal{N}(0, \sigma_\varepsilon^2)$ and $\mathcal{N}(0, \sigma_u^2)$ distributions, respectively, while $(x_i, \varepsilon_j, u_k)^\top$ are mutually independent for all $i, j, k = 1, \ldots, n$ ("$\top$" indicates the transpose). From these assumptions, the observations $(X_i, Y_i)^\top$ are independent and distributed as

$$\begin{pmatrix} X_i \\ Y_i \end{pmatrix} \sim \mathcal{N}_2 \left(\begin{pmatrix} \mu_x \\ \beta_0 + \mu_x \end{pmatrix}, \begin{bmatrix} \sigma_x^2 + \sigma_u^2 & \sigma_x^2 \\ \sigma_x^2 & \sigma_x^2 + \sigma_\varepsilon^2 \end{bmatrix} \right), \quad i = 1, \ldots, n, \tag{2}$$

where $\beta_0, \mu_x, \sigma_x^2, \sigma_u^2$ and σ_ε^2 are unknown parameters.

Frequentist and Bayesian inferences for the model parameters in (2) and other functions of them has been widely studied in previous works, see, for example, Grubbs (1983), Jaech (1985) and de Castro & Vidal (2017), among others.

Moreover, it can be seen that the model in (2) can be obtained as reparameterization of the bivariate normal distribution

$$\begin{pmatrix} X_i \\ Y_i \end{pmatrix} \sim \mathcal{N}_2 \left(\begin{pmatrix} \mu_X \\ \mu_Y \end{pmatrix}, \begin{bmatrix} \sigma_X^2 & \rho\sigma_X\sigma_Y \\ \rho\sigma_X\sigma_Y & \sigma_Y^2 \end{bmatrix} \right), \quad i = 1, \ldots, n, \tag{3}$$

with $\rho \in (-1, 1)$. Thus, the inferences for model parameters in (2) can be obtained from $\mu_X, \mu_Y, \sigma_X^2, \sigma_Y^2$ and ρ, which by solving a system of equations (given in de Castro & Vidal (2017)), it leads to the following solution:

$$\mu_x = \mu_X, \ \beta_0 = \mu_Y - \mu_X, \ \sigma_x^2 = \sigma_{XY}, \ \sigma_u^2 = \sigma_X^2 - \sigma_{XY} \text{ and } \sigma_\varepsilon^2 = \sigma_Y^2 - \sigma_{XY}, \tag{4}$$

where $\sigma_{XY} = \rho\sigma_X\sigma_Y$ and with the constraints $\sigma_{XY} > 0, \sigma_X^2 - \sigma_{XY} > 0$ and $\sigma_Y^2 - \sigma_{XY} > 0$.

On the other hand, recently published papers has involved the fiducial argument (a concept initially regarded by R.A. Fisher in 1935), which in its generalized form led to the development of the generalized fiducial inference (GFI), see Hannig *et al.* (2016). These

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authors presented a concise review of the recent advances of GFI and several applications in different statistical problems. Taking into account this approach, two generalized fiducial methods for the Grubbs model were proposed in Tomaya & de Castro (2018), which the numerical findings have shown good properties in interval estimation, especially when the sample size is small and moderate.

Now, motived by the development of a new fiducial method, in this work, we present the estimation method based on the subjective fiducial distribution proposed in Bowater & Guzmán-Pantoja (2018) for the model in (2) and we compare it with the results based on the generalized fiducial distribution (GFD) reported in Tomaya & de Castro (2018).

2 Subjective fiducial inference

In this section, we briefly present some important definitions about the subjective fiducial inference and refer to Bowater & Guzmán-Pantoja (2018), for more details and some philosophical discussions.

Suppose that a sampling model that depends on a vector of unknown parameters $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_p)^\top$ generates the data z. The joint density of the data z given the true value of $\boldsymbol{\theta}$ is denoted by $g(z|\boldsymbol{\theta})$. In the one-dimensional case, the sampling model depends on one unknown parameter θ_1, either because there are no other parameters, or because the true values of $\theta_2, \ldots, \theta_p$ are known.

Given the assumption above, a fiducial statistic $Q(z)$ is defined as being an one-dimensional sufficient statistic for θ_1 if it exits, otherwise it can be assumed to be any one-to-one function of a unique maximum likelihood (ML) estimator of θ_1.

Now, regardless of how the data was generated, it will be assumed that the data set z was generated by the following algorithm:

Step 1. To draw a value u from a continuous one-dimensional random variable U, with a probability density function (pdf) $f_U(u)$ that does not depend on the parameter θ_1.

Step 2. To determine a value $q(z)$ for a fiducial statistic $Q(z)$ by setting U equal to u and $q(z)$ equal to $Q(z)$ in the following definition of the distribution of $Q(z)$:

$$Q(z) = \varphi(U, \theta_1), \tag{5}$$

where the function $\varphi(U, \theta_1)$ is defined so that it holds the following conditions:

a) The distribution of $Q(z)$ as defined in (5) is equal to what it would have been if $Q(z)$ had been determined on the basis of the data set z.

b) The variable U is the only random variable that $\varphi(U, \theta_1)$ depends.

c) Let $G = \{u : f_U(u) > 0\}$ and let H_1 be the set of all possible values of θ_1 as specified before any information about the data z has been obtained. If it is assumed that a value for $Q(z)$ has been generated, but both its corresponding value u for the variable U and the parameter θ_1 are unknown, then substituting $Q(z)$ in equation (5) by whatever value is taken by $Q(z)$ would imply that this equation would define an injective mapping from the set G to the set H_1.

Step 3. Generate the data set z by conditioning the sampling density $g(z|\boldsymbol{\theta})$ on the already generated value for $Q(z)$.

It is worth to comment that, in the classical fiducial argument, the variable U can be seen through the fact that its distribution is the same both before and after the fiducial statistic $q(z)$ is observed.

2.1 Subjective fiducial distribution

In the case univariate, given a value $q(z)$ for the fiducial statistic $Q(z)$, the subjective fiducial distribution (SFD) of the parameter θ_1 conditional on the known parameters $\theta_2, \ldots, \theta_p$ is defined by setting $Q(z)$ equal to $q(z)$ in (5), so that the value θ_1 is treated as a realization of the random variable Θ_1, so it leads to the expression:

$$q(z) = \varphi(U, \Theta_1), \tag{6}$$

where U has a pdf $f_U(u)$ as described in Step 1 of the algorithm. Bowater & Guzmán-Pantoja (2018) pointed out that this last equation leads a valid probability distribution for the parameter θ_1 under condition (c) of Step 2.

Now, in the multivariate case, the sampling model considers all the parameters $\theta_1, \ldots, \theta_p$ as being unknown. For any given data set z, it will be assumed that the method described in the previous section allows to define the fiducial density of the parameter θ_j conditional on all other parameters $\boldsymbol{\theta}_{-j} = (\theta_1, \ldots, \theta_{j-1}, \theta_{j+1}, \ldots, \theta_p)^\top$, for $j = 1, \ldots, p$. Thus, the set of full conditional fiducial densities is denoted as

$$f(\theta_j|\boldsymbol{\theta}_{-j}, z), \quad j = 1, \ldots, p. \tag{7}$$

It well-known that if the conditional densities determine a joint distribution for the parameters $\theta_1, \ldots, \theta_p$ then this distribution must be unique. Then, based on this assumption, the conditional densities given in (7) determine a joint distribution for $\boldsymbol{\theta}$. This last distribution is defined to be the joint subjective fiducial distribution for these parameters and is denoted by $f(\boldsymbol{\theta}|z)$. Moreover, the conditional densities given in (7) do not necessarily can be expressed in analytical form.

Two principal difficulties arise from the method described above. First, there is no a result which guarantee that the full conditional fiducial densities given in (7) always determine a joint distribution for $\boldsymbol{\theta}$. Second, it can be complicated to calculated the expected value of any function of interest $h(\boldsymbol{\theta})$ with respect to the joint fiducial density of $\boldsymbol{\theta}$. However, these difficulties also is achieved with respect to posterior densities of various parameters obtained using Bayesian inference. To overcome these problems, Bowater & Guzmán-Pantoja (2018) present two distinct ways of tackling the aforementioned difficulties: an analytical method and the Gibbs sampler. These techniques will not be described here, but the Gibbs sampler is used for the next application due to its construction.

3 Applying to the Grubbs model

In this section, we first sum up the inferences about all the parameters of the bivariate normal distribution given in (3), i.e., $\mu_X, \mu_Y, \sigma_X^2, \sigma_Y^2$ and ρ, on the basis of a data set $\boldsymbol{Z} = (\boldsymbol{Z}_1^\top, \ldots, \boldsymbol{Z}_n^\top)^\top$, where $\boldsymbol{Z}_i = (X_i, Y_i)^\top$, $i = 1, \ldots, n$. Hence, the inferences on the model parameters in (2) are obtained from the measures given in (4).

Next, if μ_X is unknown being that the remaining parameters are known, a sufficient statistic for μ_X is given by $\sum_{i=1}^n X_i - \rho(\sigma_X/\sigma_Y)\sum_{i=1}^n Y_i$, which will be treated as the fiducial statistic in this case. Defining the random variable $U \sim N(0, 1)$ and by using the relationship in equation (5) allows us to define the fiducial distribution of μ_X, which is given by $\mu_X|\mu_Y, \sigma_X^2, \sigma_Y^2, \rho, \boldsymbol{Z} \sim N(\overline{X} + \rho(\sigma_X/\sigma_Y)(\mu_Y - \overline{Y}), \sigma_X^2(1-\rho^2)/n)$. Analogously, it is proceeded for μ_Y due to the symmetry of the bivariate normal distribution, i.e., the fiducial distribution for μ_Y is defined as $\mu_Y|\mu_X, \sigma_X^2, \sigma_Y^2, \rho, \boldsymbol{Z} \sim N(\overline{Y} + \rho(\sigma_Y/\sigma_X)(\mu_X - \overline{X}), \sigma_Y^2(1-\rho^2)/n)$.

Now, if all parameters except σ_X^2 are known, then there is no sufficient statistic for σ_X^2 and, in this case, a fiducial statistic for σ_X^2 will be defined as the unique ML estimator of σ_X^2, which is computed from the solution of the quadratic equation for $\hat{\sigma}_X$:

$$n(1-\rho^2)\hat{\sigma}_X^2 + \rho(\hat{\sigma}_X/\sigma_Y)\sum_{i=1}^{n}(X_i-\mu_X)(Y_i-\mu_Y) - \sum_{i=1}^{n}(X_i-\mu_X)^2 = 0. \quad (8)$$

Also, it is well known that the ML estimator is asymptotically normally distributed with mean equal to the true value and variance equal to the inverse of Fisher information. In this case, the Fisher information for σ_X is $n(2-\rho)/[\sigma_X^2(1-\rho)]$, then the equation (5) is approximated as $\hat{\sigma}_X = \sqrt{\varphi(U,\sigma_X^2)} = \sigma_X + U\sigma_X[(1-\rho^2)/n(2-\rho^2)]^{1/2}$, where $\hat{\sigma}_X$ is the ML estimator of σ_X computed by equation (8) and $U \sim N(0,1)$. This approximation is based on the central limit theorem, which is used to approximate the distribution of $q(z)$. Thus, solving the last equation for σ_X, it leads to the following approximated fiducial distribution for σ_X:

$$\sigma_X = \hat{\sigma}_X \left\{1 + U[(1-\rho^2)/(2n-\rho^2 n)]^{1/2}\right\}^{-1}, \quad (9)$$

and consequently, from (9), the fiducial distribution for σ_X^2 can be obtained. Again due to the symmetry of the bivariate normal distribution, the construction for σ_Y^2 is made in a similar way to σ_X^2, which the approximate fiducial distribution for σ_Y^2 would be as in (9) replacing σ_X and $\hat{\sigma}_X$ by σ_Y and $\hat{\sigma}_Y$, respectively, where $\hat{\sigma}_Y$ is the ML estimator of σ_Y.

Lastly, if ρ is unknown, while remaining parameters are known, following on a similar way to σ_X^2, the equation (5) is approximated by

$$\hat{\rho} = \rho + U(1-\rho^2)/\sqrt{n(1+\rho^2)}, \quad (10)$$

where $\hat{\rho}$ is the ML estimator of ρ and $U \sim N(0,1)$. Substituting a random value of U into equation (10) will lead a unique solution for ρ in which it will be regarded as random value of ρ from its approximate fiducial distribution.

In order to draw samples from the joint subjective fiducial distribution of the quantities given in (4), we take advantage of samplers developed for the parameters model in (3) applying the Gibbs sampler.

4 Simulation results and an application

In this section, a simulation study is reported to asses the performance of the point estimators for proposed procedure, as well as interval estimation in terms of the empirical coverage probability (CP) and average interval length (IL). Recall SFD is estimation method using the subjective fiducial distribution. We generate 1000 random samples of size n = 10, 20, 30 and 50 from the model described in Section 1. The data $\boldsymbol{Z}_i$ are generated from (2) with the true values of parameters: $\beta_0 = 0.220$, $\mu_x = 4.400$, $\sigma_x^2 = 0.035$, $\sigma_u^2 = 0.010$ and $\sigma_\varepsilon^2 = 0.034$. The computational implementation was developed in the R language R Core Team (2017).

Table 1: Empirical coverage probability (CP) and average interval length (IL) of the confidence intervals with confidence coefficient of 95% from the GFD and SFD methods.

		CP		IL			CP		IL	
n	Parameter	GFD	SFD	GFD	SFD	Parameter	GFD	SFD	GFD	SFD
10	μ_x	0.952	0.944	0.289	0.272	σ_u^2	0.976	0.963	0.070	0.064
20		0.955	0.948	0.196	0.191		0.977	0.946	0.042	0.039
30		0.955	0.951	0.158	0.155		0.971	0.949	0.033	0.030
50		0.949	0.954	0.121	0.119		0.970	0.940	0.025	0.022
10	σ_x^2	0.942	0.902	0.086	0.067	σ_ε^2	0.985	0.947	0.126	0.082
20		0.951	0.909	0.059	0.050		0.951	0.932	0.068	0.052
30		0.957	0.938	0.049	0.041		0.963	0.944	0.053	0.043
50		0.951	0.937	0.037	0.032		0.962	0.932	0.038	0.033

Based on 1000 replications, numerical findings showed that the average of the point estimates (the medians), the sampling standard deviation and the root mean squared error for the SFD method were very similar to those results obtained by the generalized fiducial distribution (GFD) reported in Tomaya & de Castro (2018), which they were not presented here by space limitation.

On the other hand, Table 1 displays the performance of the interval estimators. With respect to μ_x, we can observe that both methods have coverage probabilities close to level nominal (0.95), which the SFD method stands out for having slightly shorter length. With respect to σ_x^2, it can be seen that the GFD method outperforms the SFD method in terms of coverage probability that is the closest to the nominal. With respect to σ_u^2, the SFD method yields good coverage probabilities close to the nominal value even for small and moderate sample sizes and shorter interval lengths. With respect to σ_ε^2, the SFD method has good coverage probability and average interval length when $n = 10$, but the GFD method stands out for $n > 10$.

4.1 Example.(Methods comparison study) The real data set for illustrating the proposed methodology was extracted from (Jaech, 1985, Section 3.2). The results were obtained from an assay comparison study involving two methods for measuring the density of 43 cylindrical nuclear reactor fuel pellets of sintered uranium. The first method is called geometric method, which consists of weighing the pellet and finding its volume and thus obtaining the density, while the immersion method uses the change of the weight of the pellet when it is weighed in the air and in a certain liquid. Here, the measurements obtained from the geometric and immersion methods are represented by X_i and Y_i, respectively, for $i = 1, \dots, 43$. Each measurement was expressed as the percentage theoretical density minus 90% for convenience.

Table 2: The 95% confidence intervals and their lengths from the GFD and SFD methods.

	μ_x		σ_x^2		σ_u^2		σ_ε^2	
Method	Interval	Length	Interval	Length	Interval	Length	Interval	Length
GFD	[4.331, 4.463]	0.132	[0.019, 0.059]	0.040	[0.001, 0.028]	0.027	[0.020, 0.062]	0.042
SFD	[4.332, 4.462]	0.130	[0.020, 0.056]	0.036	[0.001, 0.026]	0.025	[0.020, 0.056]	0.036

In this example, the point estimates for the mean of the quantity of interest (μ_x), the product variability (σ_x^2) and the precision parameters (σ_u^2 and σ_ε^2), obtained by the SFD method, were equal to 4.4, 0.035, 0.010 and 0.034, respectively. This estimates agree with the point estimates reported in Tomaya & de Castro (2018) by the GFD method. Figures (a)–(d) show the progression of one run of 100 000 cycles of the Gibbs sampler in terms of the parameters of interest. The histograms in Figures (e)–(h) were formed on the basis of all samples of μ_x, σ_x^2, σ_u^2 and σ_ε^2.

Table 2 shows the confidence intervals and their lengths with confidence coefficient of 95% for the parameters of interest. The SFD method has the shorter interval length than the GFD method, but the simulation results in the previous section shows that the GFD method has a good performance of coverage probability, especially for σ_x^2 and σ_ε^2.

5 Conclusion

A new fiducial estimation method based on the subjective fiducial distribution was presented for the Grubbs model. Within of our study, the SFD method presented similar results to GFD method, especially for μ_x and $\sigma^2 u$.

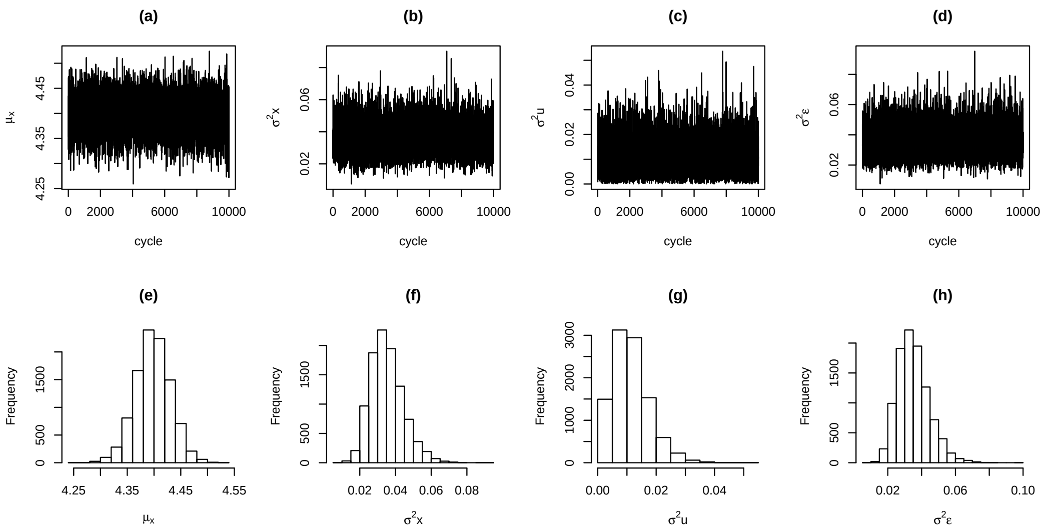

Figure 1: Gibbs sampling of the joint fiducial distribution of the parameters of interest for the Grubbs model

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