

Exact Confidence Intervals by Simulation

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1. Introduction

Suppose T is a statistic with a distribution which depends on a single unknown parameter θ . If T is stochastically increasing in θ , then it is well known how to construct an exact or conservative confidence interval for θ . For example, an upper α -confidence point when t is the observed value of T is obtained by solving the equation $F(t; \theta) = \alpha$ with respect to θ .

In the present paper we discuss how appropriate generalizations and modifications of the above idea can be used to derive exact confidence intervals. Our points of departure are the papers by Lillegård and Engen (1999) and Bølviken and Skovlund (1996). In the following these papers are referred to as, respectively, LE and BS. The basic assumption in these papers is that there is a random vector U with a known distribution, and a function $\tau(u, \theta)$ such that T under θ has the same distribution as $\tau(U, \theta)$, for each possible θ . LE treats the case when $\tau(u, \theta)$ is strictly increasing in θ , and for each pair u, t there is a unique solution $\hat{\theta}(u, t)$ for θ of the equation $\tau(u, \theta) = t$. This excludes, however, the possibility of having a $\tau(u, \theta)$ with jumps or a $\tau(u, \theta)$ which is not everywhere increasing. The method in BS basically includes the above possibilities, but is often more difficult to use than the method of LE. We shall show how one may in a certain sense unify and generalize the approaches of LE and BS.

2. The general method

Even if we do not require $\tau(u, \cdot)$ to be non-decreasing in θ , we shall at least for intuition assume that large values of T are associated with large values of θ . For example this is natural if T is an estimator for θ . For brevity we shall restrict attention to upper confidence limits. The derivation of lower limits is similar.

Define $\bar{\theta}(u, t) = \sup\{\theta : \tau(u, \theta) \leq t\}$. Suppose we want an upper α confidence bound for θ . Let $a(t)$ be the smallest number such that $P_U(\bar{\theta}(U, t) \geq a(t)) \leq \alpha$. Note that $a(t)$ is non-decreasing in t . Define $a^{-1}(\theta) = \sup\{t : a(t) \leq \theta\}$. We claim that $a(T)$ is an upper α confidence bound (possibly conservative) for θ . This is seen from

$$\begin{aligned} P_\theta(\theta \geq a(T)) &\leq P_\theta(T \leq a^{-1}(\theta)) = P_U(\tau(U, \theta) \leq a^{-1}(\theta)) \\ &\leq P_U(\bar{\theta}(U, a^{-1}(\theta)) \geq \theta) \leq \alpha \end{aligned}$$

where the second last inequality follows from the definition of $\bar{\theta}(u, t)$ while the last inequality follows from the definition of $a(t)$.

We note that if T is binomially distributed with success probability θ and $\tau(U, \theta)$ is appropriately defined, then the above approach leads to the well known Clopper-Pearson intervals. In general the result may be used for Monte Carlo computations of upper confidence bounds as follows: Let t be the observed value of T . Simulate a large number of independent realizations of U and compute the corresponding $\bar{\theta}(U, t)$. Then $a(t)$ is approximately obtained as the upper α th quantile of the empirical distribution of the simulated $\bar{\theta}(U, t)$.

Moreover, by a slight modification of the idea of LE we can prove the following result which guarantees an exact bound: Let U_1, U_2, \dots, U_m be independent realizations of U and let $\bar{\theta}_{(1)}(t) \leq \bar{\theta}_{(2)}(t) \leq \dots \leq \bar{\theta}_{(m)}(t)$ be the ordering of the values $\bar{\theta}(U_j, t)$ ($j = 1, \dots, m$). Then $\bar{\theta}_{(m-k+1)}(T)$ is an exact upper $(k/(m+1))$ -confidence bound for θ in the sense that for all θ ,

$$P_{\theta}(\theta > \bar{\theta}_{(m-k+1)}(T)) \leq \frac{k}{m+1} \quad (1)$$

To prove this, note first that we can write $T = \tau(U_0, \theta_0)$ where θ_0 is the true value of θ and U_0 is an unobserved realization of U . By definition of $\bar{\theta}(u, t)$ it is seen that $\theta > \bar{\theta}(u, t)$ implies $\tau(u, \theta) > t$. It follows that the event $\theta_0 > \bar{\theta}_{(m-k+1)}(T)$ implies the event that at least $m - k + 1$ of the values $\tau(U_i, \theta_0)$ ($i = 1, \dots, m$) exceed $T \equiv \tau(U_0, \theta_0)$. But since $\tau(U_0, \theta_0), \tau(U_1, \theta_0), \dots, \tau(U_m, \theta_0)$ are $m + 1$ i.i.d. random variables, the latter event has probability $k/(m+1)$. This proves (??).

We remark that under the stronger requirements on $\tau(u, \theta)$ as used in LE, the event $\theta > \bar{\theta}(u, t)$ is equivalent to $\tau(u, \theta) > t$. The above proof then holds with equality in (??) and we obtain the main result of LE.

REFERENCES

- Bølviken, E. and Skovlund, E. (1996). Confidence intervals from Monte Carlo tests. *Journal of the American Statistical Association*, **91**, 1071-1078.
- Lillegård, M. and Engen, S. (1999). Exact confidence intervals generated by conditional parametric bootstrapping. *Journal of Applied Statistics*, **26**, 447-459.

RESUME

Cet article discute comment obtenir des limites exactes de confiance pour un paramètre θ , par simulation fondée sur une statistique T . Le méthode est fondé sur une représentation de T sur θ par $\tau(U, \theta)$, où la distribution de U soit connue.