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New results for computing exact confidence intervals for one parameter discrete distributions

Bruno LECOUTRE[1] and Jacques POITEVINEAU[2]

[1]*ERIS, Laboratoire de Mathématiques Raphael Salem, CNRS-Université de Rouen Avenue de l'Université, BP 12, 76801 Saint-Etienne-du-Rouvray, France. bruno.lecoutre@univ-rouen.fr*
[2]*ERIS and UMR 7190, IJLRA/LAM/LCPE, C.N.R.S., Université Paris 6 et Ministère de la Culture, 11 rue de Lourmel, 75015 Paris, France. jacques.poitevineau@upmc.fr*

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Abstract: The authors state new general results for computing exact confidence interval limits for usual one-parameter discrete distributions. Specific results for implementing an accurate and fast algorithm are made explicit for the binomial, negative binomial, Poisson and hypergeometric model.

Résumé: Les auteurs établissent de nouveaux résultats généraux pour calculer les limites d'un intervalle de confiance exact pour les distributions discrètes à un paramètre usuelles. Des résultats spécifiques pour implémenter un algorithme précis et rapide sont explicités pour les modèles binomial, binomial négatif, de Poisson.

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1. INTRODUCTION

An *exact* $100(1-\alpha)\%$ confidence interval method guarantees that its coverage rate never falls below the nominal confidence level $1-\alpha$. For a binomial proportion for instance, the Clopper-Pearson (1934) confidence interval is an early and popular exact method. It is the only method that also guarantees that the one-tailed probability of error is at most $\alpha/2$, both for the lower and upper limits. This interval, however, can lead to very conservative inferences. It can be excessively wide and its coverage rate may be substantially greater than $1-\alpha$.

Various attempts have been made for implementing "optimal" exact confidence intervals for one parameter discrete distribution: see especially Sterne (1954), Crow (1956), Blyth & Still (1983), Casella (1986), Blaker (2000, 2001), Kabaila & Byrne (2001), Hirji (2006). However these intervals are rarely used in practice. A first reason is that they require very intensive computations and are not always available for moderately large sample sizes. A second reason is that they have undesirable, pathological, properties. So, the Sterne method may yield two separate intervals rather than one. This is also the case for the "simple improved" procedure proposed by Cai & Krishnamoorthy (2005). The Blyth-Still-Casella and Kabaila and Byrne intervals may violate the natural *nesting condition*: if $\alpha < \alpha'$ then the $100(1-\alpha')\%$ confidence interval should be included in the $100(1-\alpha)\%$ interval (Blaker, 2000).

This has lead us to consider the exact confidence interval method for a discrete parameter studied in details by Blaker (2000). We will call it the Blaker interval, even if its principle was known before (e.g., Cox & Hinkley, 1974, page 79). The Blaker interval does not present the above problems, but has also some "undesirable behaviors". The most serious of them is that it fails to be a monotonic function of the sample size. For instance, if one success has been observed in a binomial sample of size n, the Blaker method gives the following 95% intervals:

$n=9$ [.0057,.4435] $n=10$ [.0051,.4444] $n=11$ [.0047,.4010]

So, if the sample size is increased from 9 to 10, and simultaneously the observed success rate is decreased from 1/9 to 1/10, this does not result in a smaller upper limit, as could be expected. The undesirable behaviors of the Blaker interval have been discussed by Vos & Hudson (2008). They are inherent to discrete distributions and are the price to pay for reducing the two-tailed probability of error of the Clopper-Pearson interval.

The original algorithm for computing Blaker's confidence limits (2000, 2001) is based on a computationally very intensive method and is very far from being optimal. In this paper, we will state new and general results that allow to implement an optimized accurate algorithm for one parameter discrete distributions. The computation time is minimized, so that the interval can be easily computed even for extremely large sample sizes. Moreover, this allows to implement an iterative procedure that systematically searches for non monotonicity and corrects it. The resulting exact confidence interval is appropriate for situations where a coverage at least as large as $1-\alpha$ must be guaranteed.

The paper will be organized as follows. Section 2 describes the Blaker interval and the shortcomings of the original algorithm. Section 3 makes explicit general assumptions for a discrete distribution indexed by a real-valued parameter. Then new results for finding the Blaker's confidence limits under these assumptions are stated. Section 4 gives some numerical illustrations and comments. A simple correction for non-monotonicity is proposed. Section 5 states that the above assumptions are satisfied for the usual binomial, negative binomial and Poisson models. For each model, the specific results for implementing an efficient algorithm are given. The hypergeometric model serves to illustrate the case of an integer parameter. Proofs are given in Appendix.

2. EXACT BLAKER'S CONFIDENCE INTERVALS

Consider the same situation as in Blaker (2000). Let a statistic X have a discrete distribution indexed by a real-valued parameter θ and let U^* denote the upper limit of the $100(1-\alpha)\%$ Blaker's confidence interval for θ associated with the observation $X=x$. Note that the lower limit L^* can be computed as the upper limit for an appropriate transformed parameter, for instance $1-\theta$ or $1/\theta$. Consequently, we will restrict our attention to the computation of the upper limit.

Let $p_\theta(x)$ denote the probability mass function of X and

$$P_\theta(x) = \Pr_\theta(X \leq x)$$

denote its cumulative distribution function. Assume that X is stochastically increasing, i.e. $P_\theta(x)$ is decreasing in θ for all x.

Let again

$$P^*_\theta(y) = \Pr_\theta(X \geq y) = 1 - P_\theta(y-1)$$

and for any integer y such that $y > x+1$, consider the sum and the difference

$$\Xi(\theta,x,y) = P_\theta(x) + P^*_\theta(y) \quad \text{and} \quad \Delta(\theta,x,y) = P_\theta(x) - P^*_\theta(y).$$

Note that for all θ, $\Xi(\theta,x,x+1)=1$, so that the case $y=x+1$ will be irrelevant, and consequently excluded in the following. This concerns in particular the case in which X has a maximum finite value x_{max} and $x = x_{\text{max}}$. It follows that U^* is the maximum possible value θ_{max} of θ_0.

2.1. The exact upper limit

Consider the one-tailed test of $H_0: \theta = \theta_0$ against $H_1: \theta < \theta_0$ based on X. For the observed value x, the P-value of this test is $P_{\theta_0}(x)$. Define $U_{\alpha/2}$ the upper limit of the $100(1-\alpha)\%$ equal-tailed confidence interval for θ based on inverting the above test, i.e. the largest accepted θ_0. It can be computed by solving

$$P_{U_{\alpha/2}}(x) = \tfrac{1}{2}\alpha.$$

It is an exact upper limit in the sense that for all θ, $1 - P_\theta(U_{\alpha/2})$, the probability that θ exceeds $U_{\alpha/2}$, is at most $\alpha/2$.

2.2. The upper limit of the Blaker interval

The upper limit U^* of the $100(1-\alpha)\%$ Blaker's interval is based on inverting the following one-tailed test of $H_0 : \theta = \theta_0$ against $H_1 : \theta < \theta_0$. Define the "acceptability function" $\bar{\alpha}(\theta_0, x)$ of this test as

$$\bar{\alpha}(\theta_0, x) = \min\{\Xi[\theta_0, x, x^*(\theta_0, x)], 1\}$$

where $x^*(\theta_0, x)$ is the smallest integer y such that $y \geq x$ and $P^*_{\theta_0}(y) \leq P_{\theta_0}(x)$, i.e. $\Delta(\theta_0, x, y) \geq 0$. Note that when $P_{\theta_0}(x) = P^*_{\theta_0}(x)$ then $x^*(\theta_0, x) = x$ and $\bar{\alpha}(\theta_0, x) = 1$.

The Blaker upper limit U^* is the largest value accepted by the test at level α, i.e. such that $\bar{\alpha}(\theta_0, x) \geq \alpha$. This ensures that U^* is included between the exact one-tailed upper limits U_α $[P_{U_\alpha}(x) = \alpha]$ and $U_{\alpha/2}$ $[P_{U_{\alpha/2}}(x) = \alpha/2]$.

Blaker (2000, 2001) proposed an algorithm that computes the limit by successive decrements. Starting from $\theta_0 = U_{\alpha/2}$, the hypothesized value is decremented by a small amount ϵ (which controls the precision) while $\bar{\alpha}(\theta_0, x) < \alpha$. This algorithm, based on a computationally intensive method, is very far from being optimal. In particular, each decrement needs to compute a quantile function. Substantial numerical precision can only be achieved with very small ϵ-decrements and is hardly attainable in practice. Moreover, the algorithm may fail (see Klaschka, 2010) when ϵ is not sufficiently accurate. For instance, for the binomial distribution, if 2 successes have been observed for a sample size of 123, the Blaker S-Plus function returns the right value 0.0575 for $\epsilon = .00001$ but 0.0552 for $\epsilon = .0001$.

In the case of the binomial distribution, Klaschka (2010) developed an alternative algorithm, free of most of the drawbacks of the above algorithm. However, it does not avoid computing a non negligible number of quantile functions. Moreover, this algorithm is based on results specific to the binomial distribution and is not available for other distributions.

3. NEW RESULTS AND PROCEDURE

Remark that

$$\Xi(\theta_0, x, y) = \bar{\alpha}(\theta_0, x)$$

if and only if $y = x^*(\theta_0, x)$, i.e.

$$P^*_{\theta_0}(y) \leq P_{\theta_0}(x) < P^*_{\theta_0}(y-1) \Leftrightarrow \Delta(\theta_0, x, y) \geq 0 \text{ and } \Delta(\theta_0, x, y-1) < 0.$$

The principle of our algorithm is to use this equivalence, in order to avoid the unnecessary computation of quantiles. Consider the following situation.

3.1. Assumptions

Assumption 1. *Assume that $P_\theta(x)$ is a strictly decreasing continuous function of θ. It follows that $P^*_\theta(y)$ is a non decreasing continuous function of θ. This implies that the difference $\Delta(\theta, x, y)$ is a strictly decreasing function of θ. An immediate consequence is that it exists a unique value $\widetilde{\theta}(x, y)$, such that*

$\Delta[\widetilde{\theta}(x,y),x,y]=0$.

When X has a maximum finite value $x_{\max}$, it may occur that $P^*_\theta(y)=0$ for all θ, so that $\Xi(\theta,x,y)=\Delta(\theta,x,y)=P_\theta(x)$. For instance, for the binomial distribution $\text{Bin}(n,\theta)$, $x_{\max}=n$ and when $\Pr_{U_{\alpha/2}}(X=n)>P_{U_{\alpha/2}}(x)$ then $x^*(U_{\alpha/2})=n+1$, which implies to consider the case $y=n+1$, for which $P^*_\theta(n+1)=0$ for all θ.

Assumption 2. *Excluding the above particular case, assume that the sum $\Xi(\theta,x,y)$ ($y>x+1$) has a unique minimum for $\breve{\theta}(x,y)$ and that it is a strictly decreasing continuous function when $\theta<\breve{\theta}(x,y)$ and a strictly increasing continuous function when $\theta>\breve{\theta}(x,y)$.*

The above situation is illustrated in Figure 1 for a binomial distribution with $n=20$, $x=5$ and $y=14$. The proof that the binomial distribution satisfies the two assumptions is given in Section 5.1. The half sum $\Xi(\theta_0,5,14)/2$ is displayed for more clarity. The minimum is attained for $\breve{\theta}(5,14)=.4735$, close to $\widetilde{\theta}(5,14)=.4740$ (which is a general result).

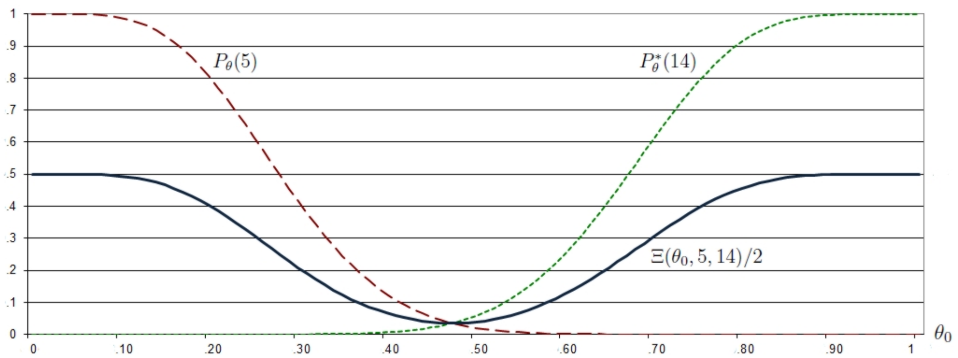

FIGURE 1: Illustration: binomial distribution with $n=20$, $x=5$, $y=14$, $P_\theta(5)$, $P^*_\theta(14)$ and $\Xi(\theta_0,5,14)/2$ as a function of θ_0.

3.2. Fundamental results

The algorithm must include a procedure for determining $x^*(U^*,x)$. In what follows, we show that $x^*(U^*,x)$ can only take one of the two values $x^*(U_{\alpha/2},x)$ or $x^*(U_{\alpha/2},x)-1$. Recall that $U_\alpha\le U^*\le U_{\alpha/2}$ and let $x^+=x^*(U_{\alpha/2},x)$, $x^-=x^*(U_\alpha,x)$ and $x^*=x^*(U^*,x)$, so that $x^-\le x^*\le x^+$. If assumptions 3.1 and 3.1 are satisfied, then the two following propositions hold.

Proposition 1. *It exists a unique value $\theta_\alpha\in[U_\alpha,U_{\alpha/2}]$ such that $\Xi(\theta_\alpha,x,x^+)=\alpha$. Moreover, If $\Delta(\theta_\alpha,x,x^+-1)<0$ then $x^*=x^+$ and $U^*=\theta_\alpha$. In the particular case $\Xi(\theta,x,y)=P_\theta(x)$ for all θ, $U^*=U_\alpha$.*

Proposition 2. *If $x^- < x^+$, it exists a unique value $\widetilde{\theta} \in [U_\alpha, U_{\alpha/2}[$ such that $\Delta(\widetilde{\theta}, x, x^+ - 1) = 0$. If $\Xi(\widetilde{\theta}, x, x^+) < \alpha$ then $x^* = x^+ - 1$ and $U^* = \widetilde{\theta}$.*

3.3. A simple procedure for computing U^*

For a given distribution, satisfying assumptions 1 and 2, compute U_α, $U_{\alpha/2}$ and x^+. Determine the value $\breve{\theta}(x, x^+)$ for which $\Xi(\theta_0, x, x^+)$ is minimum. In the particular case $\Xi(\theta, x, y) = P_\theta(x) = 1$ (if it exists), $U^* = \theta_{\text{max}}$. In the particular case $\Xi(\theta, x, y) = P_\theta(x)$, $U^* = U_\alpha$.

Otherwise, the upper limit is computed from the starting values α, U_α, $U_{\alpha/2}$, x, x^+, $\breve{\theta}(x, x^+)$ and the relevant characteristics of the distribution (for instance n for the binomial). If $x^- < x^+$ – i.e. $\Delta(U_\alpha, x, x^+ - 1) > 0$ – the equality $\Delta(U^*, x, x^+ - 1) = 0$ is solved on the interval $[U_\alpha, U_{\alpha/2}]$. Then if $\Xi(U^*, x, x^+) < \alpha$, $x^* = x^+ - 1$ and this gives the solution. Otherwise, $x^* = x^+$ and the equality $\Xi(U^*, x, x^+) = \alpha$ is solved on the interval $[U_\alpha, \min\{\breve{\theta}(x, x^+), U_{\alpha/2}\}]$, which is such that the function $\Xi(U^*, x, x^+)$ is strictly decreasing. The desired accuracy is achieved by successive approximations until $|\Delta(U^*, x, x^+ - 1)|$ or $|\Xi(U^*, x, x^+) - \alpha|$ is less than a fixed value δ.

4. NUMERICAL RESULTS AND COMMENTS

From Figure 2, the algorithm can be illustrated in the binomial case, for $n = 20$ and $x = 5$. For $\alpha = .05$, $U_{.05} = .4556$ and $U_{.025} = .4910$, with $x^+ = 15$.

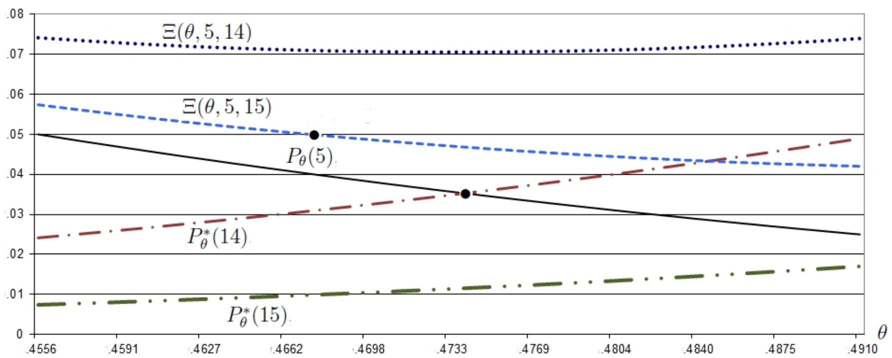

FIGURE 2: Illustration: for $n = 20$, $x = 5$ and $\alpha = .05$, hence $x^+ = 15$, the following values are plotted as a function of θ: $P_\theta(5)$, $P^*_\theta(15)$, $\Xi(\theta, 5, 15)$, $P^*_\theta(14)$, $\Xi(\theta, 5, 14)$.

4.1. Numerical illustrations

Within the limits $[.4556, .4910]$, the sum $\Xi(\theta_0, 5, 15)$ strictly decreases from .0574 to .0420, being equal to .05 for $\theta_{.05} = .4673$. Note that the minimum of $\Xi(\theta_0, 5, 15)$, which is .4139, is attained outside the limits for $\breve{\theta}(5, 15) = .5 >$

$.4910$. The difference $\Delta(.4673, 5, 14) = +0.0303$ is positive, hence the condition $\Delta(\theta_\alpha, x, x^+ - 1) < 0$ of Proposition 1 is not satisfied.

It exists a unique value $\tilde{\theta} = .4740 > .4673$ such that $\Delta(.4740, 5, 14) = 0$ (i.e. $P_\theta(5) = P^*_\theta(14)$). Since $\Xi(.4740, 5, 15) = 0.0468$ is smaller than .05, the condition $\Xi(\tilde{\theta}, x, x^+) < \alpha$ of Proposition 2 is satisfied. It follows that for $x^* = 14$ and $U^* = \tilde{\theta} = .4740$. Note that the sum $\Xi(\theta, 5, 14)$ is always greater than .05, with the minimum value 0.0705 attained for $\breve{\theta}(5, 14) = .4735$.

4.2. Undesirable behaviors

Figure 2 allows to illustrate some of the undesirable behaviors of the Blaker interval. It can be easily verified that, for all $\alpha \in [\Xi(.4740, 5, 15), \Xi(.4740, 5, 14)] = [.046823, .070542]$, $x^* = 14$, so that the same limit $U^* = \tilde{\theta} = .4740$ is obtained. Consequently, the limit is not strictly monotonic in the confidence level. A related result is that the limit is discontinuous in the confidence level at some points (See Blaker, 2000, Corollary 1, page 786). So, for $\alpha > .070543$, $U_{\alpha/2} = 0.4739884 > \tilde{\theta} = .4739888$. Consequently, the equality $\Delta(\theta_0, 5, 14) = 0$ cannot be satisfied within the limits $[U_\alpha, U_{\alpha/2}]$. It results that, for $\alpha = .070543$, $x^* = 15$ and the limit is $U^* = .4731$, given by $\Xi(U^*, 5, 15) = .070543$. Nevertheless, the Blaker interval satisfies the nesting condition: if $\alpha < \alpha'$ then the $100(1 - \alpha')\%$ confidence interval is always included in (eventually equal to) the $100(1 - \alpha)\%$ interval.

When the limit U^* is the solution $\tilde{\theta}$ of $\Delta(\theta_0, x, x^+ - 1) = 0$ ($x^* = x^+ - 1$), due to the U-shaped form of the Ξ function, it may exist two values such that $\Xi(\theta_0, x, x^+) = \alpha$ that are both smaller than $\tilde{\theta}$ (even if it is not the case in our example). This implies that the Blaker interval may contain values such that $\bar{\alpha}(\theta_0, x) < \alpha$, which are consequently rejected by the acceptability function.

4.3. A simple correction for non-monotonicity

As emphasized in introduction, the most serious undesirable property of the Blaker interval in the case of the binomial model is that U^* may be a non-monotonic function of the sample size. Our fast algorithm allows for systematically searching and identifying non-monotonicities for a given x, by computing the limit for $n + 1, n + 2, \ldots$ So, for the 505 000 upper limits of all 95% binomial confidence intervals obtained for n varying from 1 to 1000, 1 080 cases of non-monotonicities were found. Then a simple correction can be applied. If, for given x and n, a larger limit is found for x and $n + k$, it is taken as the limit for x and all sample size from n to $n + k$. The search process can be stopped when $U_{\alpha/2}$ for $n + k$ is smaller than the larger Blaker limit previously found. The coverage rate of the resulting corrected for non-monotonicity interval is virtually unchanged. For instance, if one success has been observed for a sample size of 295, the upper limit of the Blaker 95% interval is .01759. It decreases until 313 (.0166) and increases for 314 (.01762). Consequently, the upper limit is changed to .01762 for all n from 295 to 313.

Note that systematic searches with the negative binomial and Poisson models have revealed no case of non-monotonicity. For the hypergeometric model, non-monotonicities only occur for sufficiently large population size N, when the sampling distribution is close to the binomial distribution. So, for $x = 1$, the upper limit for the number of events in the population is smaller for $n = 10$ than for $n = 9$ when $N \leq 2722$, while these two limits are respectively 1205 and 1210 when $N = 2723$.

5. SPECIFIC RESULTS FOR SOME USUAL SAMPLING MODELS

We will give here all the practical results needed for implementing our algorithm for the binomial, negative binomial, Poisson and hypergeometric models.

5.1. Binomial model

Let X_i $(i = 1, \ldots n)$ be independent Bernoulli random variables having the same parameter θ. Define $X = \sum_{i=0}^{n} X_i$, X has a binomial distribution $\text{Bin}(n, \theta)$. Due to the relationship between the binomial and beta cumulative distribution functions (Johnson, Kemp & Kotz, 1993, page 117), the following equalities hold

$$P_\theta(x) = \Pr_\theta(X \leq x) = B_{n,\theta}(x) = 1 - IB_\theta(x+1, n-x)$$

$$P^*_\theta(y) = \Pr_\theta(X \geq y) = 1 - P_\theta(y-1) = 1 - B_{n,\theta}(y-1)$$
$$= IB_\theta(y, n-y+1),$$

where $B_{n,\theta}(x)$ denotes the binomial cumulative distribution function and $IB_\theta(a,b)$ is the regularized incomplete beta function. It results that for $0 \leq x < n$, $P_\theta(x)$ is a strictly decreasing from 1 (for $\theta = 0$) to 0 (for $\theta = 1$) continuous function of θ. In practice $U_{\alpha/2}$ and U_α can be computed from the inverse incomplete beta function. For instance, $U_{\alpha/2} = IB^{-1}_{1-\alpha/2}(x+1, n-x)$.

The particular case $x = n$, for which $U^* = U_{\alpha/2} = 1$, can be excluded. The value x^+ associated with $U_{\alpha/2}$ can be computed from the quantile function of the binomial distribution as $x^+ = B^{-1}_{n,U_{\alpha/2}}(1 - \alpha/2) + 1$. The value $\breve{\theta}(x, x^+)$ is given by the following lemma.

Lemma 1. *Assuming $0 \leq x < n-1$ and $x+1 < y \leq n$, the sum $\Xi(\theta, x, y)$ is a continuous U-shaped function, varying from 1 (for $\theta = 0$) to 1 (for $\theta = 1$). Its minimum is attained for*

$$\theta = \frac{\rho}{1+\rho} \quad \textit{where } \rho = \left(\frac{B(y, n-y+1)}{B(x+1, n-x)}\right)^{1/(y-x-1)} = \left(\frac{\Gamma(y)\Gamma(n-y+1)}{\Gamma(x+1)\Gamma(n-x)}\right)^{1/(y-x-1)}.$$

In the particular case $x^+ = n+1$, compute $\Pr_{U_\alpha}(X = n)$. If $\Pr_{U_\alpha}(X = n) \geq \alpha$, then $U^* = U_\alpha$. Note that when $x = n-1$, which implies $x^+ = n+1$, $\Pr_{U_\alpha}(X = n) = \alpha$. Otherwise, compute U^* following the procedure given in Section 3.3. For the lower limit L^*, replace x with $n-x$ and apply the same procedure, which gives the upper limit for $1-\theta$, i.e. $1 - L^*$. This result follows from the equalities

$$P_{1-\theta}(n-x) = P^*_\theta(x) = 1 - IB_{1-\theta}(n-x+1, x)$$

$P^*_{1-\theta}(n-y) = P_\theta(y) = IB_{1-\theta}(n-y, y+1)$.

5.2. Negative Binomial model

Consider a series of independent Bernoulli random variables X_i having the same parameter θ. let T be the number of non-events before s events are observed with probability θ. T has a negative binomial distribution.

For the upper limit, consider $X = -T$. Due to the relationship between the negative binomial and beta cumulative distribution functions (Johnson, Kemp & Kotz, 1993, page 210), the following equalities hold ($x \leq 0, y \leq 0$)

$P_\theta(x) = \mathrm{Pr}_\theta(X \leq x) = \mathrm{Pr}_\theta(T \geq -x) = 1 - NB_{s,\theta}(-x-1)$
$= 1 - IB_\theta(s, -x)$

$P^*_\theta(y) = \mathrm{Pr}_\theta(X \geq y) = \mathrm{Pr}_\theta(T \leq -y) = 1 - P_\theta(y-1) = NB_{s,\theta}(-y)$
$= IB_\theta(s, -y+1)$.

where $NB_{n,\theta}(x)$ denotes the negative binomial cumulative distribution function. It results that $P_\theta(x)$ is a strictly decreasing from 1 (for $\theta = 0$) to 0 (for $\theta = 1$) function of θ. In practice $U_{\alpha/2}$ and U_α can be computed from the inverse incomplete beta function. For instance, $U_{\alpha/2} = IB^{-1}_{1-\alpha/2}(s, -x)$.

The particular case $x = 0$, for which $U^* = U_{\alpha/2} = 1$, can be excluded. The value x^+ associated with $U_{\alpha/2}$ can be computed from the quantile function of the negative binomial distribution as $x^+ = -NB^{-1}_{s,U_{\alpha/2}}(\alpha/2) + 1$. The value $\breve{\theta}(x, x^+)$ is given by the following lemma.

Lemma 2. *Assuming $x < -1$ and $x + 1 < y \leq 0$, the sum $\Xi(\theta, x, y)$ is a U-shaped continuous function, varying from 1 (for $\theta = 0$) to 1 (when $\theta = 1$). Its minimum is attained for*

$$\theta = 1 - \left(\frac{B(s,-y+1)}{B(s,-x)}\right)^{1/(x-y+1)} = 1 - \left(\frac{\Gamma(-y+1)\Gamma(s-x)}{\Gamma(-x)\Gamma(s-y+1)}\right)^{1/(x-y+1)}.$$

In the particular case $x^+ = 1$, compute $\mathrm{Pr}_{U_\alpha}(X = 0)$. If $\mathrm{Pr}_{U_\alpha}(X = 0) \geq \alpha$, then $U^* = U_\alpha$. Note that when $x = -1$, which implies $x^+ = 1$, $\mathrm{Pr}_{U_\alpha}(X = 0) = \alpha$. Otherwise, compute U^* following the procedure given in Section 3.3.

For the lower limit L^*, consider $X = T$. Then $P_\theta(x)$ and $P^*_\theta(y)$ can be expressed as functions of $1-\theta$ ($x \geq 0, y > x$)

$P_\theta(x) = \mathrm{Pr}_\theta(T \leq x) = NB_{s,1-(1-\theta)}(x) = 1 - IB_{1-\theta}(x+1, s)$
$P^*_\theta(y) = \mathrm{Pr}_\theta(T \geq y) = 1 - NB_{s,1-(1-\theta)}(y-1) = IB_{1-\theta}(y, s)$.

It results that $P_\theta(x)$ is a strictly decreasing continuous function of $1-\theta$. It can be verified as previously that $\Xi[\theta, x, y]$ is a continuous U-shaped function of $1-\theta$. Its minimum is attained for

$$1 - \theta = \left(\frac{B(y,s)}{B(x+1,s)}\right)^{1/(x-y+1)} = \left(\frac{\Gamma(y)\Gamma(s+x+1)}{\Gamma(x+1)\Gamma(s+y)}\right)^{1/(x-y+1)}.$$

Consequently, the upper limit for $1-\theta$ is equal to $1 - L^*$.

Since in this case X has no maximum value, there is no particular case to consider. Compute $L_{\alpha/2}$ and L_α (the upper limits for $1-\theta$) from the inverse incomplete beta function, for instance $L_{\alpha/2} = IB^{-1}_{1-\alpha/2}(x+1,s)$. Compute x^+ as $NB^{-1}_{n,1-L_{\alpha/2}}(1-\alpha/2)+1$, and follow the procedure given in Section 3.3 with the appropriate values for computing the upper limit of $1-\theta$.

5.3. Poisson model

Let X_i $(i = 1, \dots n)$ be independent Poisson random variables having the same parameter θ. Define $X = \sum_{i=0}^{n} X_i$, X has a Poisson distribution Pois$(n\theta)$.

Due to the relationship between the Poisson and gamma cumulative distribution functions (Johnson, Kemp & Kotz, 1993, page 160), the following equalities hold

$$P_\theta(x) = \Pr_\theta(X \leq x) = Poi_{n\theta}(x) = 1 - IG_{n\theta}(x+1)$$
$$P^*_\theta(y) = \Pr_\theta(X \geq y) = 1 - P_\theta(y-1) = 1 - Poi_{n\theta}(y-1) = IG_{n\theta}(y)$$

where $Poi_{n\theta}(.)$ denotes the Poisson cumulative distribution and $IG_\theta(k)$ is the regularized incomplete gamma function. It results that $P_\theta(x)$ is a strictly decreasing from 1 (for $\theta = 0$) to 0 (when $\theta \to \infty$) function of θ. In practice $U_{\alpha/2}$ and U_α can be computed from the inverse incomplete gamma function. For instance $U_{\alpha/2} = IG^{-1}_{1-\alpha/2}(x+1)/n$.

The value x^+ associated with $U_{\alpha/2}$ can be computed from the quantile function of the Poisson distribution as $x^+ = Poi^{-1}_{nU_{\alpha/2}}(1-\alpha/2)+1$. The value $\breve{\theta}(x,x^+)$ is given by the following lemma.

Lemma 3. *Assuming* $0 \leq x$ *and* $x+1 < y$*, the sum* $\Xi(\theta,x,y)$ *is a U-shaped continuous function, varying from 1 (for* $\theta = 0$*) to 1 (when* $\theta \to \infty$*). Its minimum minimum is attained for*

$$\theta = \frac{1}{n}\left(\frac{\Gamma(y)}{\Gamma(x+1)}\right)^{1/(y-x-1)}.$$

Compute U^* following the procedure given in Section 3.3.There is no particular case to consider.

For the lower limit L^*, consider $X = -\sum_{i=0}^{n} X_i$. Then $P_\theta(x)$ and $P^*_\theta(y)$ can be expressed as functions of $1/\theta$ $(x < 0, x < y \leq 0)$

$$P_\theta(x) = \Pr_\theta(-X \geq x) = 1 - Poi_{n/(1/\theta)}(-x-1) = 1 - IG^{\text{inv}}_{(1/\theta)/n}(-x)$$
$$P^*_\theta(y) = \Pr_\theta(-X \leq y) = Poi_{n/(1/\theta)}(-y) = IG^{\text{inv}}_{(1/\theta)/n}(-y+1)$$

where $IG^{\text{inv}}_{(1/\theta)/n}(k) = 1 - IG_{n\theta}(k)$ is the regularized incomplete inverse gamma function. It results that $P_\theta(x)$ is a strictly decreasing continuous function of $1/\theta$. It can be verified as previously that $\Xi[\theta,x,y]$ $(x < -1, x+1 < y \leq 0)$ is a continuous U-shaped function of $1/\theta$. Its minimum is attained for

$$\frac{1}{\theta} = n\left(\frac{\Gamma(-x)}{\Gamma(-y+1)}\right)^{1/(x-y-1)}.$$

Consequently, the upper limit for $1/\theta$ is equal to $1/L^*$.

Compute $L_{\alpha/2}$ and L_α (the inverse of the upper limits for $1/\theta$) from the inverse incomplete gamma function, for instance $L_{\alpha/2} = IG^{-1}_{\alpha/2}(-x+1)/n$. The particular case $x = 0$, for which $L^* = L_{\alpha/2} = 0$, can be excluded. The value x^+ associated with $L_{\alpha/2}$ can be computed from the quantile function of the Poisson distribution as $x^+ = -Poi^{-1}_{nL_{\alpha/2}}(\alpha/2) + 1$. In the particular case $x^+ = 1$, compute $\Pr_{L_\alpha}(X = 0)$. If $\Pr_{U_\alpha}(X = 0) \geq \alpha$, then $U^* = U_\alpha$. Note that when $x = -1$, which implies $x^+ = 1$, $\Pr_{U_\alpha}(X = 0) = \alpha$. Otherwise, use the procedure given in Section 3.3 with the appropriate values for computing the upper limit of $1/\theta$.

5.4. Hypergeometric model

Consider a finite population of size N that contains M events and $N - M$ non-events. Let X be the number of events in a sequence of n draws without replacement. X has an hypergeometric distribution with parameter M

$$Pr_M(X = x) = \frac{\Gamma(M+1)\Gamma(N-M+1)\Gamma(n+1)\Gamma(N-n+1)}{\Gamma(x+1)\Gamma(M-x+1)\Gamma(n-x+1)\Gamma(N-M-n+x+1)\Gamma(N+1)}.$$

Due to the relationships between the hypergeometric, negative hypergeometric and beta-binomial cumulative distribution functions (Johnson, Kemp & Kotz, 1993, pages 254-255), the following equalities hold

$$P_M(x) = \Pr_M(X \leq x) = HG_{N,n,M}(x) = 1 - BB_{x+1,n-x,N-n}(M - x - 1)$$

$$P^*_M(y) = \Pr_M(X \geq y) = 1 - P_M(y - 1) = 1 - HG_{N,n,M}(y - 1)$$
$$= BB_{y,n-y+1,N-n}(M - y),$$

where $HG_{N,n,M}(x)$ and $BB_{a,b,K}(t)$ respectively denote the hypergeometric and beta-binomial (that replaces the beta) cumulative distribution functions. In this form $\theta = 1/M$ ($0 \leq \theta \leq 1$) can be considered as a real-valued parameter (even if in practice it can take only a finite number of values). Then the upper and lower limits for θ can be computed in the same way as for the binomial model. However, in practice, the confidence limits for the discrete parameter M can be computed by a very simple procedure. In this case, the equalities $\Xi(\theta_0, x, x^+) = \alpha$ and $\Delta(\theta_0, x, x^+ - 1) = 0$ are replaced with inequalities. Starting from $U = U_{\alpha/2}$ (an integer value), decrement U until either $\Xi(U, x, x^+ - 1) \geq \alpha$ and $\Delta(U, x, x^+ - 1) \geq 0$ or $\Xi(U, x, x^+) \geq \alpha)$ and $\Delta(U, x, x^+ - 1) \leq 0$.

CONCLUDING REMARKS

FORTRAN and R codes implementing our algorithm are available upon requests to the authors. We have favored simplicity and robustness. Some improvement in speed could be achieved by refining the code. For all models, our algorithm was systematically investigated, for various values of α. The accuracy parameter δ was set to 10^{-6}, 10^{-9} and 10^{-12}. The results were compared to the original Blaker algorithm with the decrement $\epsilon = .0001$. This decrement was diminished only in case of discrepancy. Following this procedure, all results agree with four decimal places.

For the binomial model, our algorithm was compared to the Klaschka one. The confidence limits were calculated for all intervals when n varied from 1 to

1000 (501 500 intervals) for various values of α and δ. Both algorithms gave the same results within the required precision. The execution times were comparable, slightly smaller for our algorithm, and similar to those given in Klaschka (2010, Table 4.1).

APPENDIX

Proof of Proposition 1. Two cases are to be considered.
(i) If $\Xi(\theta, x, x^+) > P_\theta(x)$ for all θ, the following inequalities hold

$$\Xi(U_\alpha, x, x^+) = \alpha + P^*_{U_\alpha}(x^+) > \alpha$$
$$\Delta(U_\alpha, x, x^+) = \alpha - P^*_{U_\alpha}(x^+) > 0$$

and, because $0 < P^*_{U_{\alpha/2}}(x^+) \leq \alpha/2$,

$$\Xi(U_{\alpha/2}, x, x^+) = \tfrac{1}{2}\alpha + P^*_{U_{\alpha/2}}(x^+) \leq \alpha$$
$$\Delta(U_{\alpha/2}, x, x^+) = \tfrac{1}{2}\alpha - P^*_{U_{\alpha/2}}(x^+) \geq 0.$$

The U-shaped form of Ξ implies the existence and unicity of θ_α. Moreover, for any hypothesized value θ_0 such that $\theta_\alpha < \theta_0 \leq U_{\alpha/2}$, $\Xi(\theta_0, x, x^+) < \alpha$. If $\Delta(\theta_\alpha, x, x^+ - 1) < 0$ then

$$\bar{\alpha}(\theta_\alpha, x) = \Xi(\theta_\alpha, x, x^+) = \alpha \text{ and } \Delta(\theta_0, x, x^+ - 1) < \Delta(\theta_\alpha, x, x^+ - 1) < 0.$$

Since $\bar{\alpha}(\theta_0, x) = \Xi(\theta_0, x, x^+) < \alpha$, θ_0 is rejected and consequently $x^* = x^+$ and $U^* = \theta_\alpha$. Note that $\Xi(\breve{\theta}(x, x^+), x, x^+) \leq \alpha$, which implies that $U^* \leq \min[\breve{\theta}(x, x^+), U_{\alpha/2}]$.
(ii) If $\Xi(\theta_0, x, x^+) = P_{\theta_0}(x)$ for all $\theta_0 \in [U_\alpha, U_{\alpha/2}]$, then $\Xi(\theta_0, x, x^+) < \alpha$, except for U_α: $\Xi(U_\alpha, x, x^+) = \alpha$. It results that $\theta_\alpha = U_\alpha$.

■

Proof of Proposition 2. The existence and unicity of $\widetilde{\theta}$ follows from the two following inequalities. Because $0 < P^*_{U_\alpha}(x^+ - 1) \leq \alpha$ (which is a consequence of the inequality $x^- < x^+$),

$$\Delta(U_\alpha, x, x^+ - 1) = \alpha - P^*_{U_\alpha}(x^+ - 1) \geq 0$$

and, because $P^*_{U_{\alpha/2}}(x^+ - 1) > \alpha/2$,

$$\Delta(U_{\alpha/2}, x, x^+ - 1) = \tfrac{1}{2}\alpha - P^*_{U_{\alpha/2}}(x^+ - 1) < 0.$$

The inequality $\Delta(\widetilde{\theta}, x, x^+) > 0$ (see Proposition 1) implies that $\bar{\alpha}(\widetilde{\theta}, x) = \Xi(\widetilde{\theta}, x, x^+ - 1)$. Since $\Xi(\widetilde{\theta}, x, x^+ - 1) = 2P^*_{\widetilde{\theta}}(x^+ - 1) > 2P^*_{U_{\alpha/2}}(x^+ - 1) > \alpha$, $\widetilde{\theta}$ is smaller than U^*. Moreover, assuming $\Xi(\widetilde{\theta}, x, x^+) < \alpha$, any θ_0 such that $\theta_0 > \widetilde{\theta}$ is rejected by the $\bar{\alpha}$ acceptability function, either because $\Xi(\theta_0, x, x^+) < \alpha$ (due the U-shaped form of Ξ), or because $\Delta(\theta_0, x, y) \leq \Delta(\widetilde{\theta}, x, y) < 0$ for any $y < x^+$.

It follows that U^* is the largest $\theta_0 \in [U_\alpha, U_{\alpha/2}]$ such that either $\Xi(\theta_0, x, x^+ - 1) \geq \alpha$ and $\Delta(\theta_0, x, x^+ - 1) = 0$ or $\Xi(\theta_0, x, x^+) = \alpha$ and $\Delta(\theta_0, x, x^+ - 1) \geq 0$.

■

Proof of Lemma 1. The result follows from the derivative of

$$\Xi[\theta, x, y] = 1 - IB_\theta(x+1, n-x) + IB_\theta(y, n-y+1)$$
$$= 1 - \frac{1}{B(x+1,n-x)} \int_0^\theta v^x (1-v)^{n-x-1} dv + \frac{1}{B(y,n-y+1)} \int_0^\theta v^{y-1}(1-v)^{n-y} dv,$$

which is $\Xi' = -\frac{1}{B(x+1,n-x)}\theta^x(1-\theta)^{n-x-1} + \frac{1}{B(y,n-y+1)}\theta^{y-1}(1-\theta)^{n-y}$. ■

Proof of Lemma 2. The result follows from the derivative of

$$\Xi[\theta, x, y] = 1 - IB_\theta(s, -x) + IB_\theta(s, -y+1)$$
$$= 1 - \frac{1}{B(s,-x)} \int_0^\theta v^{s-1}(1-v)^{-x-1} dv + \frac{1}{B(s,-y+1)} \int_0^\theta v^{s-1}(1-v)^{-y} dv,$$

which is $\Xi' = \frac{1}{B(s,-y+1)}\theta^{s-1}(1-\theta)^{-y} - \frac{1}{B(s,-x)}\theta^{s-1}(1-\theta)^{-x-1}$. ■

Proof of Lemma 3. The result follows from the derivative of

$$\Xi[\theta, x, y] = 1 - IG_{n\theta}(x+1) + IG_{n\theta}(y)$$
$$= 1 - \frac{1}{\Gamma(x+1)} \int_0^{n\theta} v^x \exp(-v) dv + \frac{1}{\Gamma(y)} \int_0^{n\theta} v^{y-1} \exp(-v) dv$$

which is $\Xi' = \frac{1}{\Gamma(y)}(n\theta)^{y-1} \exp(-n\theta) - \frac{1}{\Gamma(x+1)}(n\theta)^x \exp(-n\theta)$.

■

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R Code

This section gives the R code for computing Blaker's confidence limits. We have favored simplicity and robustness. Some improvement in speed could be achieved by refining the code.

1. The function "upperlimit"

The function "upperlimit" is common to all real-valued parameters.

```
upperlimit <- function(alpha,epsilon,u1,u2,thetamin,x,xp,arg){
  # is $x^- < x^+$, i.e. $\Xi(U_\alpha, x, x^+ - 1) > 0$ ?
  pq <- sumdif(u1,arg,x,xp-1)
  if (pq[2]>0){
  # solve $\Delta(U^*, x, x^+ - 1) = 0$
    umin <- u1
    umax <- u2
    pq[2] <- 1
    while (abs(pq[2])>epsilon){
      u <- (umin + umax)/2
      pq <- sumdif(u,arg,x,xp-1)
      if (pq[2]>0) {umin <- u} else {umax <- u} }
    pq <- sumdif(u,arg,x,xp)
    if (pq[1]¡alpha) return(u)}
  # solve $\Xi(U^*, x, x^+) = \alpha$
  umin <- u1
  umax <- min(u2,thetamin)
  pq[1] <- 2
  while (abs(pq[1]-alpha)>epsilon){
    u <- (umin + umax)/2
    pq <- sumdif(u,arg,x,xp)
    if (pq[1]>alpha) {umin <- u} else {umax <- u}}
  return(u)}
```

2. The function "sumdif"

The function "sumdif" is specific to each model, for instance, for the upper limit of the Poisson parameter.

```
sumdif <- function(theta,arg,x,y){
    #$P_\theta(x) = \Pr_\theta(X \le x)$
    p <- ppois(x,arg*theta)
    #$P^*_\theta(y) = \Pr_\theta(X \ge y) = 1 - P_\theta(y-1)$
    q <- 1-ppois(y-1,arg*theta)
    #return $\Xi(\theta, x, y)$ and $\delta(\theta, x, y)$
    sumdif <- c(p+q,p-q)}
```

For the other cases, use the appropriate instructions for computing p and q, for instance for the lower limit of the Poisson parameter

p <- 1-ppois(-x-1,arg/theta)
q <- ppois(-y,arg/theta)

3. The specific main functions

For each model, use appropriate main functions, for instance for the Poisson parameter (this can be easily generalized to other models).

bpoissonsup <- function(epsilon,alpha,x,n)
#*compute the uper limit of the Poisson parameter*
#*compute* U_α *and* $U_\alpha/2$
u1 <- qgamma(1-alpha,x+1)/n
u2 <- qgamma(1-alpha/2,x+1)/n
#*compute* x^+
xp <- qpois(1-alpha/2,n*u2)+1
#*compute the value of* θ *for which* $\Xi(\theta, x, x^+)$ *is minimum*
thetamin <- exp((lgamma(xp)-lgamma(x+1))/(xp-x-1)-log(n))
#*use the function "upperlimit"*
u <- upperlimit(alpha,epsilon,u1,u2,thetamin,x,xp,n)
return(u)
bpoissoninf <- function(epsilon,alpha,x,n){
#*compute the lower limit of the Poisson parameter*
#*particular case* $x = 0$
if (x==0) return(0)
#*compute* L_α *and* $L_\alpha/2$
l1 <- qgamma(alpha,x)/n
#*particular case* $x = 1$
if (x==1) return(l1)
l2 <- qgamma(alpha/2,x)/n
#*compute* x^+
xp <- qpois(alpha/2,n*l2)+1
#*particular case* $x^+ = 1$
if (xp==1){
p <- dpois(0,n*l1)
if (p>alpha) return(l1)}
#*compute the value of* $1/\theta$ *for which* $\Xi(\theta, x, x^+)$ *is minimum*
if (xp < 1)
{invthetamin <- exp((lgamma(x)- lgamma(-xp + 1))/(-xp - x + 1) + log(n))
else {invthetamin <- 1/l1}
#*use the function "upperlimit"*

```
    u <- upperlimit(alpha,epsilon,1/l1,1/l2,invthetamin,-x,xp,n)
    return(1/u)}
```

4. A specific function for the hypergeometric model

The function “bhyperG” computes the upper limit of the hypergeometric parameter by successive decrements. The quantile function of the beta-binomial distribution, which gives $U_\alpha/2$, is not directly available, but can be computed from the qghyper function in the SuppDists package.

```
bhyperG <- function(epsilon,alpha,x,N,n){
    #particular case $x = n$
    if (x==n) return(N)
    #compute $U_\alpha/2$
    u2 <- x+qghyper(1-alpha/2,-x-1,N-n,-n-1)
    #compute $x^+$
    xp <- qhyper(1-alpha/2,u2,N-u2,n)+1
    #successive decrements
    repeat{
     #compute $P_\theta(x) = \Pr_\theta(X \leq x)$
      p <- phyper(x,u2,N-u2,n)
     #compute $P^*_\theta(x^+ - 1) = \Pr_\theta(X \geq x^+ - 1) = 1 - P_\theta(x^+ - 2)$
      q1 <- 1-phyper(xp-2,u2,N-u2,n)
     #compute $P^*_\theta(x^+) = \Pr_\theta(X \geq x^+) = 1 - P_\theta(x^+ - 1)$
      q <- 1-phyper(xp-1,u2,N-u2,n)
     #test the condition $\Xi(U, x, x^+ - 1) \geq \alpha$
     # and $\Delta(U, x, x^+ - 1) \geq 0$ or $\Xi(U, x, x^+) \geq \alpha)$ and $\Delta(U, x, x^+ - 1) \leq 0$
      xi <- p+q
      xi1 <- p+q1
      delta1 <- p-q1
      if ((xi1 >= alpha && (delta1 >= 0 || x+xp-1==n) )
         || (xi >= alpha && delta1 ¡= 0)) return(u2)}
      u2 <- u2-1}}
```