Confidence Intervals for the binomial parameter p

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1 Introduction

First, here is some notation for binomial probabilities. Let X be the number of successes in n independent trials with probability p of success on each trial. Let $q \equiv 1-p$. Then we know that $EX = np$, the variance of X is npq where $q = 1-p$, and so the basic variance when $n = 1$ (Bernoulli distribution) is pq. For $k = 0, 1, ..., n$,

$$P(X = k) \; = \; b(k, n, p) \; := \; \binom{n}{k} p^k q^{n-k}$$

where $:=$ means "equals by definition." Let

$$B(k, n, p) \; := \; P(X \leq k) \; = \; \sum_{j=0}^{k} b(j, n, p),$$

$$E(k, n, p) \; := \; P(X \geq k) \; = \; \sum_{j=k}^{n} b(j, n, p).$$

Clearly $B(n, n, p) \equiv E(0, n, p) \equiv 1$. $B(k, n, p)$ can be evaluated in R as pbinom(k, n, p). Thus $E(k, n, p)$ would be $1-$ pbinom$(k-1, n, p)$ for $k \geq 1$.

As functions of three variables, the binomial probabilities B and E are hard to tabulate. Rice, Table 1 in Appendix B, gives a table of $B(k, n, p)$ for $n = 5, 10, 15, 20$, and 25, and $p = .01, .05, .1, .2, ..., .9, .95$, and .99, giving B to three decimal places. There is a table of E making up a whole book of over 500 pages, published in 1955, covering values of n up to 1000, but a relatively sparse selection, e.g. for $n \geq 500$, $n = 500, 550, 600, ..., 950, 1000$. Values of p are $k/100$ for $k = 1, 2, ..., 99$ and some other rational values. Clearly, it's better to compute binomial probabilities as needed rather than to use tables.

When can binomial probabilities be well approximated by others depending on fewer parameters? Here are some well known approximations that you may recall from a probability course. If $0 < \lambda < \infty$, a random variable Y is said to have a Poisson distribution with parameter λ if $P(Y = k) = e^{-\lambda}\lambda^k/k!$ for all $k = 0, 1, \ldots$.

1. *If npq is large, then the binomial random variable X has approximately a normal distribution with its mean np and variance npq.*
2. *If n is large but npq is not, then either p is small, in which case X has approximately a Poisson distribution with parameter $\lambda = np$, or q is small, in which case $n - X$ is approximately Poisson with parameter $\lambda = nq$.*

If neither p nor q is small and n is large, then npq is large and we have the normal approximation. If n is not large, then neither a normal nor a Poisson approximation works well. For purposes of giving confidence intervals, specifically approximate 95% or 99% intervals, one can tabulate endpoints $a(X) = a(X, n)$ and $b(X) = b(X, n)$, as will be done for all $n \leq 19$ and $0 \leq X \leq n$ in a table at the end of this handout.

Next here are some definitions. For a family of probability distributions P_θ depending on a parameter θ, we may have a vector parameter such as $\theta = (\mu, \sigma)$ or (μ, σ^2) for the family of normal distributions $N(\mu, \sigma^2)$. Or, we may have a scalar parameter such as p for the binomial distribution with a given n. Suppose we want to find confidence intervals for a real-valued function $g(\theta)$, where usually $g(\theta) = \theta$ for a scalar parameter. For normal distributions we've done that for the three functions $g(\theta) = \mu$, σ^2, and σ.

In general, an *interval estimator* for $g(\theta)$ is a pair of real-valued statistics $a(X)$ and $b(X)$ such that $a(X) \leq b(X)$ for all possible observations X. Let P_θ denote probability when θ is the true value of the parameter.

1.1 Coverage probabilities

The *coverage probability* for a given interval estimator $[a(\cdot), b(\cdot)]$ of a function $g(\theta)$ of θ is defined for each possible θ as

$$\kappa(\theta, a(\cdot), b(\cdot)) = P_\theta[a(X) \leq g(\theta) \leq b(X)]. \quad (1)$$

For the binomial probability $\theta = p$, with $g(p) \equiv p$, the main case in this handout, we'll then have the coverage probability

$$\kappa(p, a(\cdot), b(\cdot)) \;=\; Pr_p[a(X) \le p \le b(X)], \tag{2}$$

where Pr_p denotes probability when p is the true value of the binomial probability. In other words

$$\kappa(p) = \sum_{k:\ a(k) \le p \le b(k)} Pr_p(X = k),$$

where $\Pr_p(X = k) = b(k, n, p) = \binom{n}{k} p^k (1-p)^{n-k}$.

For $0 < \alpha < 1/2$ (specifically, in this handout $\alpha = 0.05$ or 0.01), I will say that an interval estimator $[a(\cdot), b(\cdot)]$ is a *precise* $1 - \alpha$ or $100(1-\alpha)\%$ *confidence interval* for θ if the coverage probability exactly equals $1 - \alpha$ for all θ. As we've seen, for normal distributions $N(\mu, \sigma^2)$, and $n \ge 2$ i.i.d. observations, there are precise confidence intervals for the variance σ^2 based on χ^2 distributions, and precise confidence intervals for the mean based on t distributions. But for the binomial case there are no precise confidence intervals. The binomial random variable X has just $n+1$ possible values $0, 1, ..., n$, so for any interval estimator, there are just $n+1$ possible values $a(j)$ of the left endpoint and $b(j)$ of the right endpoint for $j = 0, 1, ..., n$. The coverage probability will take a jump upward as p crosses from below to above each $a(j)$ and downward as it crosses each $b(j)$ (unless possibly some $a(i)$ and $b(j)$ coincide). So the coverage probability in general is not constant and is not even a continuous function of p.

I'll say that an interval estimator $[a(\cdot), b(\cdot)]$ is a *secure* $1-\alpha$ or $100(1-\alpha)\%$ *confidence interval* for θ if the coverage probability is always at least $1 - \alpha$,

$$\kappa(\theta, a(\cdot), b(\cdot)) \;\ge\; 1 - \alpha \tag{3}$$

for all possible θ.

Comparing with terminology often used in books and articles, the word "exact" has often been used for what I here call "secure," whereas "conservative" has been used to mean at least secure, or with a qualifier such as "overly conservative," to indicate that the coverage probabilities are excessively larger than $1 - \alpha$.

On the other hand, the authors of beginning statistics texts mainly agree on what a confidence interval is if it is precise (as defined above), but if such an interval does not exist, most seem to have in mind a relatively vague notion of an interval estimator whose coverage probabilities are as close as practicable to $1-\alpha$ for as wide a range of θ as practicable. The texts' authors evidently want the endpoints $a(\cdot)$ and $b(\cdot)$ of the intervals to be relatively easy to compute.

1.2 The plug-in interval

By far the most popular interval for the binomial p (in beginning textbooks, not necessarily among mathematical statisticians) is the one defined as follows. Let $\hat{p} := X/n$ and $\hat{q} := 1-\hat{p}$. The *plug-in* interval estimator for p is defined by

$$[\hat{p} - z_{u(\alpha)}\sqrt{\hat{p}\hat{q}/n}, \hat{p} + z_{u(\alpha)}\sqrt{\hat{p}\hat{q}/n}], \tag{4}$$

where $u(\alpha) := 1-\frac{\alpha}{2}$ and z_u is the u quantile of a standard normal distribution: if Z has a $N(0,1)$ distribution then $P(Z \leq z_u) = u$. (We already encountered $1-\frac{\alpha}{2}$ quantiles for χ^2 and t distributions in forming 2-sided $1-\alpha$ confidence intervals for σ^2 and μ for normal distributions.) A quick way to see a fault in the plug-in interval it is to see what happens when $X = 0$, when $\hat{p} = 0$, so $a(0) = 0$ (which is fine) but also $b(0) = 0$, which is very bad, because as $p > 0$ decreases down toward 0, the coverage probability $\kappa(p)$ converges to 0. Symmetrically, if $X = n$ then $\hat{q} = 0$ and $a(n) = b(n) = 1$ so $\kappa(p) \to 0$ as $p \uparrow 1$.

1.3 Clopper–Pearson intervals

The *Clopper–Pearson* $100(1-\alpha)\%$ interval estimator for p is the interval $[a(X), b(X)] \equiv [a_{CP}(X), b_{CP}(X)]$ where $a_{CP}(X) = a_{CP}(X, n, \alpha)$ and $b_{CP}(X) = b_{CP}(X, n, \alpha)$ are such that if the true p were $a_{CP}(X)$, and $0 < X \leq n$, then if V has a binomial(n,p) distribution, the probability that $V \geq X$ would be $\alpha/2$, in other words,

$$E(X, n, a_{CP}(X)) = \alpha/2. \tag{5}$$

If $X = 0$ then $a_{CP}(0) := 0$. Symmetrically, if the true p were $b_{CP}(X)$ and $0 \leq X < n$, and U has a binomial(n,p) distribution, the probability that $U \leq X$ would be $\alpha/2$, in other words,

$$B(X, n, b_{CP}(X)) \;=\; \alpha/2, \tag{6}$$

and if $X = n$ then $b_{CP}(n) := 1$.

The Clopper–Pearson confidence interval for p if $0 < X < n$ is defined in a way very analogous to the way 2-sided precise confidence intervals are for the normal μ and σ^2. This makes the Clopper–Pearson intervals intuitive, and they have been called "exact," but they are not precise.

Theorem 1 *The Clopper–Pearson intervals are secure (for $0 < \alpha < 1$), in fact their coverage probabilities $\kappa(p) > 1 - \alpha$ for all p. Moreover, for each n and α, $\inf_{0 \le p \le 1} \kappa(p) > 1 - \alpha$, i.e. for some $\delta = \delta(n, \alpha) > 0$, $\kappa(p) \ge 1 - \alpha + \delta$ for all p.*

Proof. To see that the intervals are monotone, i.e. $a_{CP}(0) = 0 < a_{CP}(1) < \cdots < a_{CP}(n) < 1$ and $0 < b_{CP}(0) < b_{CP}(1) < \cdots < b_{CP}(n) = 1$, consider for example that $E(j, n, a(j)) = \alpha/2 = E(j+1, n, a(j+1))$, so to produce equal probability, for a larger number of successes ($X \ge j+1$, vs. $X \ge j$), $a(j+1)$ must be larger than $a(j)$. The situation for the $b(j)$ is symmetrical.

For any p with $0 \le p \le 1$, let $J = J(p)$ be the smallest j such that $p \le b(j)$, and let $K = K(p)$ be the largest k such that $a(k) \le p$. The definition makes sense since $a_{CP}(0) = 0$ and $b_{CP}(n) = 1$. Then $a(K) := a_{CP}(K) \le p \le b(J) := b_{CP}(J)$. By monotonicity, $a(i) \le a(K) \le p$ for $i = 0, 1, ..., K$ and $b(i) \ge b(J)$ for $J \le i \le n$. Let X be binomial (n, p). Then from the definitions, $\Pr_p(X > K) = 0$ if $K = n$, otherwise it equals $E(K+1, n, p) < E(K+1, n, a(K+1)) = \alpha/2$ since $E(r, n, p)$ is increasing in p and $p < a(K+1)$. Symmetrically, $\Pr_p(X < J) < \alpha/2$. It follows (using $\alpha < 1$) that $J \le K$ so $p \in [a(r), b(r)]$ for all $r = J, ..., K$ by monotonicity. If $r > K$ then $a(r) > p$ by definition of $K(p)$, while if $r < J$ then $b(r) < p$ by definition of $K(p)$. Thus $p \in [a(r), b(r)]$ if and only if $J \le r \le K$, and

$$\kappa(p) = \sum_{r=J}^{K} \Pr_p(X = r) = 1 - E(K+1), n, p) - B(J-1, n, p) > 1 - \alpha/2 - \alpha/2 = 1 - \alpha,$$

where the first (second) $\alpha/2$ is replaced by 0 if $K = n$ or $J = 0$ respectively. Also, $E(k+1, n, p)$ can only approach $\alpha/2$, for the given values of $J(p)$ and $K(p)$, for $p \uparrow a(K+1)$, and $B(J-1, n, p)$ can only approach $\alpha/2$ as $p \downarrow b(J-1)$. These things cannot happen simultaneously, so $\kappa(p)$ cannot approach $1-\alpha$ and must be $\geq 1-\alpha+\delta$ for some $\delta > 0$. This finishes the proof. $\square$

The Clopper–Pearson intervals are overly conservative in that, for example, for $0 \leq p \leq b(0)$, however $b(0)$ is defined, if the left endpoints $a(j) = a_{CP}(j)$, $\kappa(p) \geq 1-(\alpha/2)$. This is illustrated in Table 0 where for $n = 20$ and $\alpha = 0.01$, $b(0) = b_{CP}(0) \doteq 0.2327$, and for $p \leq b(0)$, which holds for $p = a(j)$ for $j \leq 10$, all coverage probabilities shown are $\geq 0.995 = 1-\alpha/2$.

One might easily be tempted, if one observes $X = 0$ and notes that the resulting interval will be one-sided in the sense that $a(0) = 0$, to choose $b(0)$ such that if $p = b(0)$, the probability of observing $X = 0$ would be α, rather than $\alpha/2$ as in definition (6). That can lose the secure property, however: for example if $n = 20$ and $\alpha = 0.01$, $b(0) \doteq 0.2327$ would be replaced by the smaller $b(0) \doteq 0.2057 < a_{CP}(10)$, and we would get $\kappa(b(0)+) \doteq 0.9868$ and $\kappa(a(10)-) \doteq 0.9876$, both less than $0.99 = 1-\alpha$. Likewise, for the secure property, if $X = n$, we need to keep $a(n)$ as it is by (5) rather than replace $\alpha/2$ by α.

The coverage probability $\kappa(p)$ can be close to $1-\alpha$ if the interval between $b(J-1)$ and $a(K+1)$, which contains p, is a short one, as seen in Table 0 for $b(2) < p < a(14)$ where $\kappa(p) \doteq 0.9904$ and so the $\delta(20, 0.01)$ as defined in Theorem 1 is about 0.0004.

Table 0. Clopper–Pearson confidence intervals for $n = 20$, $\alpha = 0.01$ and their coverage probabilities: over-conservative at $a(j)$, $1 \le j \le 10$, just secure at $b(2)+$, $a(14)-$.

At each endpoint $p = a(j) = a_{CP}(j)$ or $b(j) = b_{CP}(j)$, the coverage probability has a left limit $\kappa(p-) = \lim_{r \uparrow p} \kappa(r)$ (except for $p = a(0) = 0$) and a right limit $\kappa(p+) = \lim_{r \downarrow p} \kappa(r)$ (except at $p = 1$, not shown). Actually $\kappa(p+) = \kappa(p)$ if $p = a(j)$ for some j and $\kappa(p-) = \kappa(p)$ if $p = b(j)$ for some j.

For $p < b(0)$, we have $J(p)$ as defined in the proof of Theorem 1 equal to 0, and thus the coverage probability as shown in that proof is $B(K(p), n, p) > 1 - \alpha/2 = 0.995$ in this case as seen in the table.

The table only covers endpoints $p < 0.5$, but the rest are determined by $a(n-j) = 1 - b(j)$ for $j = 0, 1, 2, 3$ and $b(n-k) = 1 - a(k)$ for $k = 0, 1, ..., 16$, and the coverage probabilities for $1/2 \le p \le 1$ would be symmetric to those shown for $p \le 1/2$.

On an interval between two consecutive endpoints, the coverage probability will be $\kappa(p) = B(K, n, p) - B(J - 1, n, p)$ as in the proof of Theorem 1. Differentiating this with respect to p, we get telescoping sums, and the derivative equals a positive function times a decreasing function of p, which is positive when p is small and negative as p approaches 1. Thus $\kappa(p)$ cannot have an internal relative minimum on such an interval, and its smallest values must be those on approaching an endpoint, which are shown in the following table.

	endpoint	$\kappa(p-)$	$\kappa(p+)$
$a(0)$	0.0000	—	1.0000
$a(1)$	0.00025	0.9950	1.0000
$a(2)$	0.0053	0.9950	0.9998
$a(3)$	0.0176	0.9950	0.9996
$a(4)$	0.0358	0.9950	0.9994
$a(5)$	0.0583	0.9950	0.9993
$a(6)$	0.0846	0.9950	0.9991
$a(7)$	0.1139	0.9950	0.9990
$a(8)$	0.1460	0.9950	0.9989
$a(9)$	0.1806	0.9950	0.9988
$a(10)$	0.2177	0.9950	0.9988
$b(0)$	0.2327	0.9979	0.9929

$a(11)$	0.2572	0.9924	0.9962
$a(12)$	0.2991	0.9942	0.9979
$b(1)$	0.3171	0.9973	0.9927
$a(13)$	0.3434	0.9925	0.9962
$b(2)$	0.3871	0.9947	0.9904
$a(14)$	0.3904	0.9904	0.9942
$a(15)$	0.4402	0.9938	0.9976
$b(3)$	0.4495	0.9976	0.9935
$a(16)$	0.4934	0.9934	0.9974

For $a(k) \leq p < a(k+1)$ and $p \leq b(0)$, $\kappa(p) = B(k, n, p) = 1 - E(k+1, n, p)$ where $E(k+1, n, p) < E(k+1, n, a(k+1)) = \alpha/2$ by (5). Thus $\kappa(p) > 1 - \alpha/2$, overshooting the desired $1 - \alpha$ as Table 0 illustrates.

1.4 Adjusted Clopper–Pearson intervals

One can adjust the endpoints by, whenever $a'(k) := a_{CP}(k, n, 2\alpha) \leq b(0)$, which will occur for $k \leq k_0$ for some $k_0 = k_0(\alpha)$, replacing $a_{CP}(k)$ by the larger $a'(k)$. Symmetrically, for these k, $b_{CP}(n - k)$ is replaced by $1 - a'(k)$. Then the intervals remain secure, but now as $p \uparrow a(k)$ for $1 \leq k \leq k_0$, $\kappa(p)$ will approach $1 - \alpha$, so the intervals are no longer overly conservative. For $k = k_1 = k_0 + 1$, for both $\alpha = 0.05$ and 0.01, there will be a further adjustment, in which $a_{CP}(k, \alpha)$, which is less than $b(0)$, will be replaced by a number just slightly less than $b(0)$ to avoid excess conservatism. These adjustments are made in Table 2 at the end.

2 Approximations to binomial probabilities and confidence intervals

As of now, the Clopper–Pearson interval endpoints can easily be computed by computers but not necessarily by calculators. In the algorithm in the Appendix, adjusted Clopper–Pearson intervals are used for $n \leq 19$ and their endpoints are tabulated for those n.

We already saw one approximate interval, the plug-in interval, based on a normal approximation. Recall again that if npq is large, then a binomial(n, p) variable X is approximately normal $N(np, npq)$.

2.1 Poisson probabilities and approximation

On the other hand if $p \to 0$ and $n \to \infty$ with $np \to \lambda$ and $0 \le \lambda < \infty$, then the binomial distribution converges to that of a Poisson(λ) variable Y, for which here are notations: for $k = 0, 1, ...$, letting $0^0 := 1$ in case $\lambda = 0$,

$$P(Y = k) = p(k, \lambda) := e^{-\lambda}\lambda^k/k!, \quad P(k, \lambda) := P(Y \le k) = \sum_{j=0}^{k} p(j, \lambda),$$

$$Q(k, \lambda) \ := \ P(Y \ge k) \ = \ \sum_{j=k}^{\infty} p(j, \lambda).$$

In R, $P(k, \lambda)$ can be evaluated as ppois(k, λ), where "pois" indicates the specific distribution and "p" indicates the (cumulative) probability distribution function, analogously as for the binomial and other distributions. One could also find $Q(k, \lambda)$ in R as $1-$ ppois($k - 1, \lambda$).

If $p \to 1$ and $n \to \infty$ with $nq \to \lambda$ then the distribution of $n - X$ converges to that of Y, Poisson(λ) ("reverse Poisson" approximation). If n is not large, then neither the normal nor the Poisson approximation to the binomial distribution is good. Similarly, as λ becomes large, the Poisson(λ) becomes approximately $N(\lambda, \lambda)$, but if λ is not large, the normal approximation to the Poisson distribution is not good.

2.2 Three-regime binomial confidence intervals

In statistics, where p is not known but X is observed, then for valid confidence intervals we need to proceed as follows. For n not large, specifically in this handout for $n \le 19$, instead of any approximation, one can just list the confidence interval endpoints in a table. I chose for this purpose adjusted Clopper–Pearson intervals, given in Table 2 in the appendix. This choice is not crucial itself, but secure intervals were chosen for the following reason. For small n, individual values of X have substantial probability. So, there will be substantial jumps in coverage probabilities when one crosses an endpoint. If one makes the coverage probabilities equal to $1 - \alpha$ on average, then at points just outside of individual intervals, they could be substantially less than $1 - \alpha$, which would be undesirable.

Similarly, if λ is not large, then individual values of Y have substantial probability, and it seemed best to use endpoints that give secure coverage probabilities $\ge 1 - \alpha$ in the region where they are used. These will be the

Poisson analogue of adjusted Clopper–Pearson endpoints and will be given in Table 1 in the appendix.

If n is large enough (here, $n \geq 20$) but the smaller of X and $n - X$ is no larger than $k_1 = k_1(\alpha)$, then it's better to choose endpoints, specifically $a(k)$ if $k \leq k_1$ or $k = n$, and $b(k)$ if $k = 0$ or $k \geq n - k_1$, based on a Poisson approximation, rather than a normal approximation. The binomial endpoints $a(k)$ for $k \leq k_1$ will be the corresponding Poisson endpoints given in Table 1, divided by n.

For other endpoints, we can use a normal approximation method, but which method? There is a competitor to the plug-in intervals for binomial confidence intervals based on a normal approximation.

2.3 Quadratic confidence intervals

One can get the *quadratic* or *Wilson* (1927) intervals as follows. The symbol "$\approx$" will mean approximately equal, or approximately having the distribution. Let $0 < p < 1$ and $q \equiv 1 - p$, If X is binomial (n, p) and npq is large enough, $X \approx \mathrm{N}(np, npq)$, $X - np \approx \mathrm{N}(0, npq)$ and for $\hat{p} = X/n$, $\hat{p} - p \approx \mathrm{N}(0, pq/n)$. For $z = z_{u(\alpha)}$ as in (4),

$$1 - \alpha \;\approx\; \Pr(|\hat{p} - p| \leq z\sqrt{pq/n}) \;=\; \Pr\left((\hat{p} - p)^2 \leq z^2 p(1-p)/n\right).$$

This is true for p in an interval having endpoints $a_Q < b_Q$ which are the two roots of the quadratic equation in p

$$(\hat{p} - p)^2 \;=\; z^2 p(1-p)/n. \tag{7}$$

If $0 < \hat{p} < 1$ then the quadratic $f(p) = (\hat{p} - p)^2 - z^2 p(1-p)/n$ satisfies $f(0) > 0$, $f(\hat{p}) < 0$, and $f(1) > 0$, so by the intermediate value theorem, $0 < a_Q < \hat{p} < b_Q < 1$. If $\hat{p} = 0$ then $a_Q = 0 < b_Q < 1$, or if $\hat{p} = 1$ then $0 < a_Q < b_Q = 1$. One can see that the quadratic interval is approximating binomial probabilities by normal ones for p at the endpoints of the interval, so that one approximates probabilities in the definition of the Clopper–Pearson interval (5), (6). Whereas, the plug-in interval crudely uses the normal approximation to the binomial at the center $p = \hat{p}$ where $\hat{p}\hat{q}$ may be quite different from pq at one or both endpoints.

2.4 Conditions for approximation of quadratic by plug-in intervals

If not only n but $n\hat{p}\hat{q} = X(n-X)/n$ is large enough, the plug-in and quadratic intervals will be approximately the same, so one can use the simpler plug-in interval. Here are some specific bounds.

Let $z := z_{u(\alpha)} = 1.96$ for $\alpha = 0.05$ and 2.576 for $\alpha = 0.01$. If the respective endpoints of the two kinds of intervals are within some $\varepsilon > 0$ of each other, then so must be their centers $(a(j) + b(j))/2$, which are $\hat{p} = X/n$ for the plug-in interval and for the quadratic interval, $(2X + z^2)/(2n + 2z^2)$, the midpoint of the two solutions of (7). The distance between the centers is thus bounded by

$$D_1 := \left|\frac{X}{n} - \frac{2X + z^2}{2n + 2z^2}\right| = \frac{z^2|2X - n|}{n(2n + 2z^2)} < \frac{z^2}{2n}. \tag{8}$$

The distance from the center to either endpoint is $z\sqrt{\hat{p}\hat{q}/n}$ for the plug-in interval and $z\sqrt{z^2 + 4X\hat{q}}/(2n+2z^2)$ for the quadratic interval, from solution of (7). The absolute difference between these is

$$D_2 = z\left|\frac{(n + z^2)\sqrt{4n\hat{p}\hat{q}} - n\sqrt{4n\hat{p}\hat{q} + z^2}}{2n(n + z^2)}\right|.$$

For any $A > 0$ and $B > 0$, $\sqrt{A} < \sqrt{A + B} < \sqrt{A} + B/(2\sqrt{A})$ by the mean value theorem and since the derivative $(d/dx)\sqrt{x}$ is decreasing. (The bound is most useful for $B << A$.) It follows that we can write $\sqrt{4n\hat{p}\hat{q} + z^2}$ as $\sqrt{4n\hat{p}\hat{q}} + \theta z^2/(4\sqrt{n\hat{p}\hat{q}})$ where $0 < \theta < 1$, and then that

$$D_2 \leq z^3 n^{-3/2} \max(\sqrt{\hat{p}\hat{q}}, 1/(8\sqrt{\hat{p}\hat{q}})).$$

The maximum just written is $\leq 1/(4\sqrt{\hat{p}\hat{q}})$, clearly for the second term, and for the first term, because $p(1 - p) \leq 1/4$ for $0 \leq p \leq 1$, attained at $p = 1/2$ only. It follows that $D_2 \leq z^3/(4n\sqrt{n\hat{p}\hat{q}})$. From this and (8), the distance between corresponding endpoints of the quadratic and plug-in intervals is bounded above by

$$D_1 + D_2 \leq \frac{z^2}{2n}\left(1 + \frac{z}{2\sqrt{n\hat{p}\hat{q}}}\right). \tag{9}$$

For $\alpha = 0.05$, taking $z = 1.96$, it will be assumed that

$$n\hat{p}\hat{q} \;=\; X(n-X)/n \;\geq\; 9,$$

which implies that $X \geq 9$ and $n-X \geq 9$, and so that a normal approximation is applicable (for $X \leq 8$ or $X \geq n-8$ the algorithm in the appendix uses Poisson approximations). It follows then that given n, the differences between endpoints are bounded above by $D_1 + D_2 \leq f(z)/n$ where $f(z) = (z^2/2)(1 + (z/6)) \leq 2.5483$ using (9) and $\sqrt{n\hat{p}\hat{q}} \geq 3$. We thus have $D_1 + D_2 \leq 10^{-m}$ for $X(n-X)/n \geq 9$ and $n \geq 2.55 \cdot 10^m$, to be applied for $m = 2, 3$, and 4. One wants at least two decimal places of accuracy in the endpoints in nearly any application (for example, political polls, which have other errors of that order of magnitude or more), and no more than 4 places seem to make sense here, where 4 places are given in the tables.

Similarly for $\alpha = 0.01$, taking $z = 2.576$, we'll assume that

$$n\hat{p}\hat{q} \;=\; X(n-X)/n \;\geq\; 15,$$

which is equivalent to $\sqrt{n\hat{p}\hat{q}} \geq \sqrt{15}$ and implies that $X \geq 15$ and $n-X \geq 15$. For $\min(X, n-X) \leq 14$, the algorithm uses a Poisson approximation. Given n, the differences between endpoints are bounded above by $D_1 + D_2 \leq g(z)/n$ where $g(z) = (z^2/2)(1 + \{z/(2\sqrt{15})\}) \leq 4.4213$ using (9) and $\sqrt{n\hat{p}\hat{q}} \geq \sqrt{15}$. We thus have $D_1 + D_2 \leq 10^{-m}$ for $X(n-X)/n \geq 15$ and $n \geq 4.43 \cdot 10^m$, to be applied for $m = 2, 3$, and 4.

So, for example, sufficient conditions for the endpoints of the plug-in and quadratic 99% confidence intervals to differ by at most 0.0001 are that $X(n-X)/n \geq 15$ and $n \geq 44,300$. If these conditions hold, there is no need to find the quadratic interval, one can just use the plug-in interval.

2.5 Brown et al.'s comparisons; an example

The papers by Brown, Cai, and DasGupta (2001, 2002) show that the coverage probabilities for various approximate 95% confidence intervals vary and may be quite different from 0.95. They show that the quadratic interval, which they (2001) call the *Wilson* interval since apparently Wilson (1927) first discovered it, is distinctly superior to the plug-in interval in its coverage properties. The plug-in interval behaves poorly not only for p close to 0 or 1:

Example. As Brown, Cai, and DasGupta (2001, p. 104, Example 2) point out, for $p = 0.5$, presumably the nicest possible value of p, for which the distribution is symmetric, and $n = 40$, the coverage probability of the 95% plug-in interval is 0.919, in other words the probability of getting an interval not containing 0.5 is larger than 0.08 as opposed to the desired 0.05. Let's look at this case in more detail. When $X = 14$, the right endpoint of the plug-in 95% confidence interval is

$$0.35 + 1.96\sqrt{0.35(0.65)/40} = 0.49781 < 0.5.$$

By symmetry since $p = 0.5$, if $X = 26$, the left endpoint of the plug-in 95% confidence interval is $1 - 0.49781 = 0.50219 > 0.5$, so 0.5 is included in the plug-in interval only for $15 \leq X \leq 25$. The probability that $X \leq 14$ is $B(14, 40, 0.5) = 0.040345$ and symmetrically the probability that $X \geq 26$ is $E(26, 40, 0.5) = 0.040345$, so the coverage probability $\kappa(1/2)$ of the plug-in interval in this case is $1 - 2(0.040345) \doteq 0.9193$, confirming Brown et al.'s statement. For the Clopper–Pearson confidence intervals, still for $n = 40$, if $X = 14$ the right endpoint of the interval is 0.51684. For the quadratic interval, it's 0.5049. So these intervals both do contain 0.5, while if $X = 13$ they don't. We have $B(13, 40, 0.5) = E(27, 40, 0.5) = 0.01924$. So the coverage probability of the Clopper–Pearson and quadratic intervals when $n = 40$ and $p = 0.5$ are both $1 - 2(0.01924) \doteq 0.9615$. This coverage probability is closer to the target value of 0.95 by a factor of about 3 relative to the plug-in interval. Also, it may be preferable to have coverage probability a little larger than the target value than to have it smaller.

This is just one case, but it illustrates how the quadratic interval is estimating variance from a value of p at its endpoint, namely 0.5049, which is close to 0.5, the true value. And this is not only by coincidence, but because 14 is the smallest value of X for which the Clopper–Pearson interval contains 0.5, so we'd like the confidence interval to contain 0.5 but not by a wide margin. Whereas, to estimate variance via plug-in, using $p = 0.35$, gives too small a value, and the interval around 0.35 isn't wide enough to contain 0.5. Then the coverage probability is too small.

Brown et al. (2001, Fig. 4) show that for nominal $\alpha = 0.01$ and $n = 20$, the coverage probability of the plug-in interval is strictly less than $1 - \alpha = 0.99$ for all p and oscillates wildly to much lower values as $\min(p, 1 - p)$ becomes small, e.g. < 0.15.

Another strange and undesirable property of the plug-in interval is that for any $\alpha < 0.3$ and all n large enough, $a(1) < 0 = a(0)$. Specifically, for the 95% plug-in interval with $n \geq 2$ we will have $a(1) < 0$ and $b(n-1) > 1$.

3 Desiderata for interval estimators of p

Some properties generally considered desirable for interval estimators $[a(X), b(X)]$ of the binomial p (e.g. Blyth and Still, 1983; Brown et al. 2001, 2002), are as follows:

1. *Equivariance.* For any $X = 0, 1, ..., n$, $a(n - X) = 1 - b(X)$, $b(n - X) = 1 - a(X)$.

All intervals mentioned in this handout are equivariant.

2. *Monotonicity.* $a(X)$ and $b(X)$ should be nondecreasing (preferably strictly increasing) functions of X and nonincreasing (preferably strictly decreasing for $X > 0$) functions of n.

We saw that the 95% (or higher) plug-in interval is not monotone when $n \geq 2$. The other intervals mentioned are all monotone.

3. *Union.* We have $\bigcup_{j=0}^{n}[a(j), b(j)] = [0, 1]$.

If the union doesn't include all of $[0, 1]$ there is some p for which $\kappa(p) = 0$, which seems clearly bad, but this doesn't seem to occur for any commonly used intervals. On the other hand for $n \geq 2$ the 95% plug-in intervals extend below 0 and beyond 1 and so violate the union assumption in a different way.

The remaining desiderata are less precise and can conflict with one another. It's desirable that the coverage probabilities should be close to the nominal $1 - \alpha$. Let's separate this into two parts:

4. *Minimum Coverage.* The minimum coverage probability should not be too much less than $1 - \alpha$.

I conjecture that the intervals to be given in the algorithm in the Appendix have $\kappa(p) \geq 1 - 1.6\alpha$ for $\alpha = 0.05$ or 0.01 and all n and p. I have not been able to prove this. I checked it by computer for n up to 600 and selected larger n.

5. *Average coverage.* The average coverage probability, namely $\int_0^1 \kappa(p, a(\cdot), b(\cdot))dp$, should be close to $1 - \alpha$ for n large enough.

6. *Shortness.* Consistently with good coverage, the intervals should be as

short as possible.

7. *Ease of use and computation.* Intervals proposed to be taught and given in textbooks should not be too complicated or difficult to compute.

Quadratic equations are easy to solve by computer especially when, as for quadratic interval endpoints, the roots are guaranteed to be real.

An even more easily computed interval is that of Agresti and Coull (1998). When $\alpha = 0.05$, it's (in one version, otherwise approximately) the modification of the plug-in interval in which n is replaced by $\tilde{n} = n + 4$ and $\hat{p}$ by $(X + 2)/\tilde{n}$, i.e. as if two more successes and two more failures are added to those actually observed. From the comparisons by Brown et al. (2001), the Agresti–Coull interval appears to have minimum coverage probabilities not much less than the nominal ones and tends to be secure for small $\min(p, q)$. Its average coverage probability exceeds the nominal one, with a slowly decreasing difference (bias). The Agresti–Coull intervals tend to be longer than those of some competing intervals whose average coverage probabilities are closer to the nominal.

4 Poisson interval estimators

We can apply a Poisson approximation to the binomial distribution when n is large (in the algorithm to be given, $n \geq 20$) and p is either small or close to 1. Since we observe X and don't know p, we need to use a criterion based on X. For $\alpha = 0.05$, a Poisson approximation will be used when $X \leq 8$, or a "reverse Poisson" approximation when $n - X \leq 8$.

First let's see how we can get confidence intervals (interval estimators) for the Poisson parameter λ itself. Let Y have a Poisson(λ) distribution where λ is unknown. We can estimate λ simply by Y (since $EY = \lambda$). Suppose for some $\alpha > 0$, specifically $\alpha = 0.05$ or 0.01, we want to get a $1 - \alpha$ confidence interval for λ. The definition of Clopper–Pearson interval extends naturally to the Poisson case. Given Y, let the upper endpoint $b_{CPP}(Y, \alpha) = b$ such that $P(Y, b) = \alpha/2$, using the notation for Poisson probabilities from Subsection 0.2.1. If $Y = 0$, let $a_{CPP}(Y) = 0$. If $Y > 0$, let $a_{CPP}(Y, \alpha) = a$ such that $Q(Y, a) = \alpha/2$.

We can also get analogues of quadratic intervals for λ based on the normal approximation for λ large enough. Namely, as λ is both the mean and the variance of the Poisson(λ) distribution, we take the quadratic equation $(Y -$

$\lambda)^2 = \lambda z_{u(\alpha)}^2$ or $g(\lambda) = (\lambda - Y)^2 - \lambda z_{u(\alpha)}^2 = 0$. Just as in the binomial case, if $0 < Y < \infty$, we have $g(0) = Y^2 > 0$, $g(\lambda) \to +\infty$ as $\lambda \to +\infty$, and $g(Y) < 0$, so there are two real roots of g,

$$0 < a_{Q,P}(Y) < Y < b_{Q,P}(Y).$$

When $Y = 0$ we also get two roots, now $a_{Q,P}(0) = 0$ and $b_{Q,P}(0) = z_{u(\alpha)}^2$.

As in the binomial case illustrated in Table 0, the Clopper–Pearson intervals will be excessively conservative in case $a_{CPP}(X, \alpha) < b(0)$, and so they will be adjusted, using $a_{CPP}(X, 2\alpha)$ instead as long as these numbers are still less than $b(0)$. Taking $b(0) = b_{Q,P}(0, \alpha)$, this occurs for $\alpha = 0.05$ when $0 \le Y \le k_0 := 7$. In the special case when $Y = k_1 = 8$, to preserve monotonicity of the endpoints and keep good coverage probabilities, $a(k_1)$ is taken to be just slightly less than $b(0)$. For $\alpha = 0.01$, making the analogous adjustment, we will have $k_0 = 13$ and $k_1 = 14$. The resulting endpoints are shown in Table 1 in the Appendix (algorithm).

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5 Appendix: Algorithm and Tables

The proposed algorithm for finding $100(1-\alpha)\%$ confidence intervals $[a(X), b(X)]$ for the binomial p when X successes are observed in n trials and $\alpha = 0.05$ or 0.01 is as follows.

1. If $n \geq 20$, go to step 2. If $n \leq 19$, use the (adjusted, cf. Subsec. 0.1.4, Clopper–Pearson) intervals given in Table 2.

2. If $n \geq 20$, then use the hybrid endpoints $a_H(X), b_H(X)$ defined as follows: if $\min(X, N - X) \leq k_1(\alpha) = 8$ for $\alpha = 0.05$ and 14 for $\alpha = 0.01$, then go to step 3. If $\min(X, n - X) > k_1(\alpha)$ then use the quadratic endpoints $a_Q(X), b_Q(X)$, specifically, letting $z := z_{u(\alpha)}$, and recalling $\hat{p} = X/n$ and $\hat{q} = 1 - \hat{p}$, given by

$$p = \frac{2X + z^2 \pm z\sqrt{z^2 + 4X\hat{q}}}{2(n + z^2)}, \tag{10}$$

where $\pm$ is $-$ for $a_Q(X)$ and $+$ for $b_Q(X)$. For $\alpha = 0.05$, using the close approximation $z \doteq 1.95996$, $z^2 \doteq 3.8414$, and for $\alpha = 0.01$, $z \doteq 2.5758$ and so $z^2 \doteq 6.6347$.

3. If $\min(X, n - X) \leq k_1(\alpha)$, recalling $k_1(0.05) = 8$ and $k_1(0.01) = 14$, and still for $n \geq 20$: if $0 \leq X \leq k_1(\alpha)$ let $a_H(X) = a_{H,P}(X)/n$ where the hybrid Poisson endpoints $a_{H,P}$ are given in Table 1. Likewise if $X \geq n - k_1(\alpha)$ let $b_H(X) = 1 - a_{H,P}(n - X)/n$. In particular $b_H(n) = 1$.

Let $b_H(0) = z^2_{u(\alpha)}/n$, recalling the approximations to $z = z_{u(\alpha)}$ and z^2 given above, Symmetrically let $a_H(n) = 1 - z^2_{u(\alpha)}/n$.

Define $a_H(X) = a_Q(X)$ as given by (10) in all other cases, namely if $k_1(\alpha) < X < n$, and $b_H(X) = b_Q(X)$ for $0 < X < n - k_1(\alpha)$.

Table 1. Poisson hybrid left endpoints

k	$a_{H,P}(k, 0.01)$	$a_{H,P}(k, 0.05)$
0	0.0000	0.0000
1	0.0101	0.0513
2	0.1486	0.3554
3	0.4360	0.8177
4	0.8232	1.3663
5	1.2791	1.9701
6	1.7853	2.6130

7	2.3302	3.2853
8	2.9061	3.8413
9	3.5075	
10	4.1302	
11	4.7712	
12	5.4282	
13	6.0991	
14	6.6346	

Table 2, $n \leq 19$. Use $a(k) \equiv 1 - b(n-k)$, $b(k) \equiv 1 - a(n-k)$ for $k > n/2$.

α		0.05		0.01	
n	k	$a(k)$	$b(k)$	$a(k)$	$b(k)$
1	0	.0000	.9500	.0000	.9900
2	0	.0000	.8419	.000	.9293
	1	.0253	.9747	.005	.9950
3	0	.000	.7076	.0000	.8290
	1	.017	.8646	.0033	.9411
4	0	.0000	.6024	.0000	.7341
	1	.0127	.7514	.0025	.8591
	2	.0976	.9024	.0420	.9580
5	0	.0000	.5218	.0000	.6534
	1	.0102	.6574	.0020	.7779
	2	.0764	.8107	.0327	.8944
6	0	.0000	.4593	.0000	.5865
	1	.0085	.6412	.0017	.7057
	2	.0628	.7772	.0268	.8269
	3	.1532	.8468	.0847	.9153
7	0	.0000	.4096	.0000	.5309
	1	.0073	.5787	.0014	.6434
	2	.0534	.7096	.0227	.7637
	3	.1288	.8159	.0708	.8577
8	0	.0000	.3694	.0000	.4843
	1	.0064	.5265	.0013	.6315
	2	.0464	.6509	.0197	.7422
	3	.1111	.7551	.0608	.8303
	4	.1929	.8071	.1210	.8790
9	0	.0000	.3363	.0000	.4450
	1	.0057	.4825	.0011	.5850
	2	.0410	.6001	.0174	.6926
	3	.0977	.7007	.0533	.7809
	4	.1688	.7880	.1053	.8539
10	0	.0000	.3085	.0000	.4113
	1	.0051	.4450	.0010	.5443
	2	.0368	.5561	.0155	.6482
	3	.0873	.6525	.0475	.7351
	4	.1500	.7376	.0932	.8091
	5	.2224	.7776	.1504	.8496
11	0	.0000	.2849	.0000	.3822
	1	.0047	.4128	.0009	.5086
	2	.0333	.5178	.0141	.6085
	3	.0788	.6097	.0428	.6933
	4	.1351	.6921	.0837	.7668
	5	.1996	.7662	.1344	.8307
12	0	.0000	.2646	.0000	.3569
	1	.0043	.3848	.0008	.4770
	2	.0305	.4841	.0128	.5729
	3	.0719	.5719	.0390	.6552
	4	.1229	.6511	.0759	.7275
	5	.1810	.7233	.1215	.7915
	6	.2453	.7547	.1746	.8254
13	0	.0000	.2471	.0000	.3347
	1	.0039	.3603	.0008	.4490
	2	.0281	.4545	.0118	.5410
	3	.0660	.5381	.0358	.6206
	4	.1127	.6143	.0695	.6913
	5	.1657	.6842	.1108	.7546
	6	.2240	.7487	.1588	.8113
14	0	.0000	.2316	.0000	.3151
	1	.0037	.3387	.0007	.4240
	2	.0260	.4281	.0110	.5123
	3	.0611	.5080	.0331	.5892
	4	.1040	.5810	.0640	.6579
	5	.1527	.6486	.1019	.7201
	6	.2061	.7114	.1457	.7766
	7	.2304	.7696	.1947	.8053
15	0	.0000	.2180	.0000	.2976
	1	.0034	.3195	.0007	.4016
	2	.0242	.4046	.0102	.4863
	3	.0568	.4809	.0307	.5605
	4	.0967	.5510	.0594	.6273
	5	.1417	.6162	.0944	.6882
	6	.1909	.6771	.1346	.7439
	7	.2127	.7341	.1795	.7949
16	0	.0000	.2059	.0000	.2819
	1	.0032	.3023	.0006	.3814
	2	.0227	.3835	.0095	.4628
	3	.0531	.4565	.0287	.5344
	4	.0903	.5238	.0554	.5991
	5	.1321	.5866	.0878	.6585
	6	.1778	.6457	.1251	.7132
	7	.1975	.7012	.1665	.7638
	8	.2465	.7535	.2117	.7883
17	0	.0000	.1951	.0000	.2678
	1	.0030	.2869	.0006	.3630
	2	.0213	.3644	.0090	.4413
	3	.0499	.4343	.0269	.5104
	4	.0846	.4990	.0519	.5732
	5	.1238	.5596	.0822	.6310
	6	.1664	.6167	.1168	.6846
	7	.1844	.6708	.1552	.7344
	8	.2298	.7219	.1971	.7807
18	0	.0000	.1853	.0000	.2550
	1	.0028	.2729	.0006	.3463
	2	.0201	.3471	.0085	.4217
	3	.0470	.4142	.0254	.4884
	4	.0797	.4764	.0488	.5492
	5	.1164	.5348	.0772	.6055
	6	.1563	.5901	.1096	.6579
	7	.1730	.6425	.1454	.7068
	8	.2153	.6924	.1844	.7526
	9	.2602	.7398	.2263	.7737
19	0	.0000	.1765	.0000	.2434
	1	.0027	.2603	.0005	.3311
	2	.0190	.3314	.0080	.4037
	3	.0445	.3958	.0240	.4682
	4	.0753	.4557	.0461	.5271
	5	.1099	.5120	.0728	.5818
	6	.1475	.5655	.1032	.6329
	7	.1629	.6164	.1368	.6809
	8	.2025	.6650	.1733	.7260
	9	.2445	.7114	.2124	.7684