# CONFIDENCE INTERVALS FOR THE COVERAGE OF LOW COVERAGE SAMPLES

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The coverage of a random sample from a multinomial population is defined to be the sum of the probabilities of the observed classes. The problem is to estimate the coverage of a random sample given only the number of classes observed exactly once, twice, etc. This problem is related to the problem of estimating the number of classes in the population. Non-parametric confidence intervals are given when the coverage is low such that a Poisson approximation holds. These intervals are related to a coverage estimator of Good (1953).

1. Introduction. Assume that a random sample of size N is drawn from a multinomial population with a perhaps countably infinite number of classes. Denote the probability that any particular observation belongs to class i by  $p_i$ , where  $\sum p_i = 1$ . The coverage, C, of the sample is defined to be the sum of the probabilities of the observed classes. Let  $X_i$  denote the number of observations of class i and let  $Y_i = 1$  if  $X_i \ge 1$  and  $Y_i = 0$  otherwise. Then the coverage, C, is given by

$$(1) C = \sum p_i Y_i.$$

This concept makes sense even if the number of classes is countably infinite. Also, if each class is equally likely, i.e.  $p_i = 1/s$  for each  $i = 1, 2, \dots, s$ , then  $C = N_d/s$ , where  $N_d = \sum_{k=1} N_k$  denotes the number of distinct classes observed, and statements about C can be converted into statements about s. Thus there is a relationship with the "unobserved species" and "author's vocabulary" problems which develop estimators for s.

The problem is to estimate C given  $\{N_k; k=1, 2, \cdots\}$  where  $N_k$  denotes the number of classes observed exactly k times and  $N = \sum_{k} k N_k$ . Good (1953) found the estimator

(2) 
$$C'' = 1 - (N_1/N)$$

for the coverage. The following results will not improve upon this point estimator, but rather will address the question of a limiting distribution and confidence intervals for C.

Robbins (1968) proved an exact relationship for E(C) similar to (2). Harris (1959) obtained an approximation,

$$E\{(C-C'')^2\} \doteq E(N_1+2N_2)/N^2,$$

under different conditions. Under (3) it is not an improvement on Robbin's "universal inequality" for the variance of C-C''. With either result, if the observed number of duplicates is small, the lower confidence limit may be 0, which is trivial, and the lack of a limiting distribution leaves the calculation of the confidence interval in doubt. The following result handles both problems. An example comparing these confidence intervals follows the theorems.

Let  $D = \sum_{k=1}^{\infty} N_k$  denote the number of classes observed at least twice. If all the  $p_i$ 's are sufficiently small, then D is approximately Poisson in distribution. This fact can be used to create confidence intervals for the coverage when few duplicates are observed. It will be shown that, under certain conditions,  $(N-1)C/2 \rightarrow_P E(D) > 0$ . Then the usual confidence

Received December, 1979; revised May, 1981.

AMS 1970 Subject Classification. Primary 62G15.

Key words and phrases. Coverage, occupancy problem, unobserved species, total probability.

interval for E(D) based on the observation of D yields a confidence interval for C. Furthermore, the result improves upon previously obtained confidence intervals if the conditions hold.

The above formulation assumes sampling with replacement. If each class,  $i, i \le s < \infty$ , when s is the number of classes in the population, is represented in the population by a finite number of elements,  $M_i$ , and a random sample is drawn without replacement by selection of each of the  $\sum_{i=1}^{s} M_i$  members with probability p, related results are obtained.

2. Theorems. In order to obtain a formal limit theorem sequences of N's and  $\{p_i\}$ 's are required, so a subscript n is implied but often suppressed for notational simplicity.

THEOREM 1. Let 
$$\{p_{in}, \sum_i p_{in} = 1; i = 1, 2, \dots\}$$
 and  $\{N_n\}$  be such that

(3) 
$$N \max p_i \to 0 \quad and \quad N(N-1) \sum_i p_i^2/2 \to m > 0.$$

Then

(i) D and  $N_2$  are asymptotically Poisson distributed with mean m, and  $\sum_{k=3} kN_k$  converges in probability to 0,

and

(ii) 
$$(N-1)C/2 \rightarrow_p m$$
.

COROLLARY 1. If  $Np_i$  is small for all i, then D is approximately Poisson distributed with mean  $m' = N(N-1) \sum p_i^2/2$  and P(D=0|N) is approximately  $e^{-m'}$ .

COROLLARY 2. Let d and  $n_1$  denote the observed values of D and  $N_1$ . If  $n_1$  is nearly N and much larger than d, an estimator for the coverage, C, is given by

(4) 
$$C' = 2d/(N-1).$$

Furthermore if (a, b) is a  $(1 - \alpha)$  confidence interval for the mean of a Poisson random variable based on a single observation d, then an approximate confidence interval for C of size  $(1 - \alpha)$  is given by

(5) 
$$2a/(N-1) \le C \le 2b/(N-1).$$

COROLLARY 3. If all s classes are equally likely  $(p_i = 1/s \text{ for all } i)$ , and if  $n_1$  is nearly N and much greater than d, an estimator, s', for s is given by

(6) 
$$s' = n_d(N-1)/2d,$$

where  $n_d$  denotes the number of distinct classes observed. Furthermore, an approximate confidence interval for s of size  $(1 - \alpha)$  is given by

(7) 
$$n_d(N-1)/2b \le s \le n_d(N-1)/2a$$

where a and b are as in (5).

COMMENTS. Although N and N-1 are asymptotic, the proof (see equation (14)) suggests that N-1 is the appropriate factor. In relatively small sample problems, such as Example 3, it performs better.

By (i) the results hold with  $N_2$  replacing D. As an approximation, however, D is preferable since the asymptotically negligible term of (14) in C corresponds approximately to the term of (13) in D that is not in  $N_2$ .

The estimator of (4) is in essential agreement with Good's result (2), since, using Theorem 1 (i),

$$1 - (N_1/N) = \sum_{k=2} kN_k/N \sim 2 \sum_{k=2} N_k/(N-1) = 2D/(N-1).$$

Unfortunately, the linear combination of  $N_k$ 's in a calculation paralleling (13) which best approximates (14) is  $\sum_{k=2} kN_k/2$ , which is not necessarily integer valued and does not satisfy the limit law that integer valued linear combinations with coefficient 1 on  $N_2$  satisfy. Good's result would suggest using  $\sum_{k=2} (k-1)N_k$ . It and  $\sum_{k=2} N_k = D$  have expectations differing from (14) by the same amount, the former overestimating it and the latter underestimating it. I have opted to use the latter because of the type of application in Example 1 where the randomness assumption is sometimes violated by groups of observations in the same class. In that case D gives less weight to the extra duplicates.

In the equally likely case of Corollary 3, a computation shows that the maximum likelihood estimator of s (Good, 1950, page 73) is asymptotic to s' of (6). Also,  $C = n_d/s$  so that an estimate or limit on C corresponds to an estimate or limit on s.

The second theorem pertains to a different formulation of the problem: suppose each class, i, is represented in a population by a finite number of elements,  $M_i$ , and a random sample is drawn without replacement from the population of  $\sum_{i=1}^{s} M_i$  members by selecting each element with probability p. Then the sample size, N, is itself random. By making p small and s large, results paralleling those of Theorem 1 may be obtained. If the  $M_i$ 's are not all very large, the effect of sampling without replacement alters the result somewhat. In this context let

$$C = \sum_{i=1}^{s} M_i Y_i / \sum_{i=1}^{s} M_i,$$

where  $Y_i$  is as in (1).

THEOREM 2. Let  $\{M_i\}$  be a fixed sequence of positive integers (not necessarily large) and let  $s \to \infty$  and  $p \to 0$  such that

$$p \sum_{i=1}^{s} M_i \to \infty$$

$$p \max_{i \le s} M_i \to 0,$$

and

(10) 
$$p^2 \sum_{i=1}^s M_i (M_i - 1)/2 \to m > 0.$$

Then

(i) D and  $N_2$  are asymptotically Poisson distributed with mean m, and  $\sum_{k=3} kN_k$  converges to 0 in probability,

and

(ii) 
$$N(C-p)/2 \rightarrow_p m$$
.

Furthermore, if  $M_i = M$  for all i,

(iii) 
$$\{M/(M-1)\}NC/2 \rightarrow_p m$$
.

REMARKS. The results of Theorem 2 can be used to give point estimates and confidence intervals for C. Also, (iii) gives us a feeling for how large the  $M_i$ 's should be to be able to disregard their effect if they are not precisely known. One obvious corollary is that if  $M_i$  is large for all i and the observed value of N is large and  $n_1$  is much larger than  $n_2$ , then the results of the previous corollaries hold. The accuracy of the approximations is, however, diminished by using N for E(N) and disregarding  $\{M_i\}$ . Note that in (ii) and (iii) and the associated corollaries, N is the proper factor and not N-1 as in Theorem 1.

This sampling approach has a further generalization. Suppose that the  $M_i$ 's are themselves i.i.d. positive integer-valued random variables, but that otherwise the context of Theorem 2 is maintained. The conclusions would hold if the hypotheses held with probability one.

THEOREM 3. The hypotheses to Theorem 2 hold with probability one if  $p \to 0$ ,  $p^2s \to m' > 0$ ,  $E(M^3)$  exists and M is not trivially always one.

#### 3. Examples.

EXAMPLE 1. Eddy (1967), in a hoard of ancient coins, found among 662 coins of the emperor Gordian III (244-249 AD) only two pairs struck from the same dies. The die varieties observed differ so minutely that numismatists are satisfied that they do not form a collection of differing varieties. Assuming, then, that the sample was random, this implies that a huge number of dies were employed in producing the coins. Numismatists would like a confidence interval for C. Theorem 3 is appropriate since the dies produced independent, identically distributed random numbers of coins. It is known that each  $M_i$  is on the order of 10,000 (Sellwood, 1963). Therefore we cite (iii) to justify using  $NC/2 \doteq$ E(D). The corollary parallel to (4), with N in place of N-1, as in all corollaries to Theorems 2 and 3, yields C = 4/662 = .00604 which is the same as (2). A bound on the variance from Robbins's "universal inequality" would be 1/(N+1) and no non-trivial lower confidence limit for C would be possible since  $(1/663)^{1/2} = .039$  is much too large. Harris's approximation (page 548)  $E\{(C-C'')^2\} \doteq E(N_1+2N_2)/N^2$  is not smaller and inappropriate under (3). But (5) gives non-trivial justified intervals for any desired confidence. For instance, a 95 per cent confidence interval of the form  $C_0 \leq C$  is given by  $.701/662 = .00106 = C_0 \le C$ . Numismatists examining this data find the coverage surprisingly low and are therefore interested in a confidence interval of the form  $C \leq C_1$ . Such a 95 per cent confidence interval is  $C \le C_1 = 12.6/662 = .0190$ . This result also differs substantially from any obtained from the naive incorrect application of a normal limit law. If it is assumed that  $p_i = 1/s$  for all i, confidence intervals for s have been obtained under assumptions other than (3). Usually a sample contains many duplicate observations and a normal limit law can be obtained as, say  $N/s \rightarrow k > 0$  ((3) implies k = 0). Results based on a normal limit law (for example, Darroch, 1958; or see Seber, 1973, Section 4.1.2) require a normal limit law for D which is not reasonable unless D is large. Of course, if D is large and yet the present hypotheses hold, the Poisson distribution is well approximated by a normal distribution and the two results coincide.

EXAMPLE 2. The calculation of  $P(D=0\,|\,N)$  when not all  $p_i$ 's are the same is the "generalized birthday problem." Gail et al (1979) noted an application to cancer research of the case when s is large and N is moderate. They obtained Corollary 1 and calculated  $P(D=0\,|\,N=40)$  when  $p_i=1/10,000$  for each i. The approximation, .924964, differs from the true value, .924869, by one digit in the fourth decimal place, accurate enough for most purposes.

Example 3. Suppose a sample of size 23 from s (unknown) equally likely classes yields no duplicates. Even in this extreme case (7) can be used to obtain a confidence interval for s (although not with an upper limit) and also a point estimator. The estimate from (6) would be  $s=\infty$ , which is not likely to be useful. This reflects the fact that the probability of no duplications is increasing in s. In that case a 50 per cent confidence point may be of some use. Choosing b such that (0, b) is a 50 per cent confidence interval yields 2b=1.386 and the point estimate  $s_{.50}=365.08$ . This is the reverse of the birthday problem. An approximate 95 per cent confidence interval of the form  $s \ge s_0$  is given by  $s \ge 84.5$ . The true 96 per cent confidence interval is  $s \ge 92$ . This and other examples show that the lower confidence bounds for s and upper bounds for s tend to be conservative.

# 4. Proofs of Theorems.

PROOF OF THEOREM 1. Let  $X_i$  denote the number of observations of class i in the sample of size N. For notational simplicity the subscripts, n, on  $X_i$ , N, and  $p_i$  are suppressed. Under (3)

(11) 
$$\sum_{j=k} j P(X_i = j) \sim k P(X_i = k)$$

uniformly in i, since

$$(k+1)P(X_i = k+1) = N(N-1) \cdot \cdot \cdot (N-k)p_i^{k+1}(1-p_i)^{N-(k+1)}/k!$$
$$= \{(N-k)p_i/(1-p_i)\}P(X_i = k).$$

By (3) the first factor can be made less than  $\varepsilon$  for all k uniformly in i for n sufficiently large. Summing from k+1 to infinity yields (11).

Now

(12) 
$$E(\sum_{k=3} kN_k) = \sum_{i} \sum_{k=3} kP(X_i = k) \sim 3 \sum_{i} P(X_i = 3)$$

$$\leq (N-2) \max p_i \sum_{i} N(N-1) p_i^2 (1-p_i)^{N-3} / 2 \to 0$$

by (3). Since  $\sum_{k=3} kN_k$  is nonnegative, by (12) it converges in probability to 0, proving part of (i).

For the other half of (i), let  $D_i = 1$  if  $X_i \ge 2$  and  $D_i = 0$  if  $X_i \le 1$ . Then  $D = \sum D_i$ , and

(13) 
$$E(D) = \sum E(D_i) = \sum P(X_i \ge 2) = \sum P(X_i = 2) + \sum P(X_i \ge 3) \\ \sim N(N-1)p_i^2(1-p_i)^{N-2}/2 \sim N(N-1)p_i^2/2 \to m,$$

where we have used (11) and (3) in the last three steps.

Note that the variables  $D_i$  are dependent. That  $N_2$  and D converge in distribution to the Poisson distribution with mean m will follow (Sevastyanov, 1972) if we show the r-dimensional joint probabilities are uniformly asymptotic to the corresponding product of the marginals.

$$\begin{split} P(X_{i_1} = X_{i_2} = \cdots = X_{i_r} = 2) / \{ P(X_{i_1} = 2) \cdots P(X_{i_r} = 2) \} \\ &= \frac{N! (1 - p_{i_1} - p_{i_2} - \cdots - p_{i_r})^{N-2r}}{(N - 2r)! \{ N(N - 1) \}^r (1 - p_{i_1})^{N-2} \cdots (1 - p_{i_r})^{N-2}} \rightarrow 1 \end{split}$$

uniformly, since  $N \max p_i \to 0$  by hypothesis. We did not need to separate out Sevastyanov's "rare" sets. This proves the result for  $N_2$ . The result for D follows from (12).

Recall the definition of C given by (1).

(14) 
$$E\{(N-1)C/2\} = \sum (N-1)p_i E(Y_i)/2$$

$$= \sum N(N-1)p_i^2 (1-p_i)^{N-1}/2 + \sum (N-1)p_i P(X_i \ge 2)/2$$

$$\sim N(N-1)p_i^2/2 \to m.$$

Also

$$Var\{(N-1)C/2\} \le \sum Var\{(N-1)p_iY_i/2\}$$

since the covariances are negative, and the right hand side is bounded above by

$$\sum_{i} N(N-1)^2 p_i^3 / 4 \le (\max_i Np_i) \sum_{i} N(N-1) p_i^2 / 4 \to 0.$$

Thus  $(N-1)C/2 \rightarrow_P m$ , and Theorem 1 is proven.

The condition that  $n_1$  is nearly N in Corollary 2 is required since  $E(N_1) = \sum P(X_i = 1)$   $\sim \sum Np_i = N \to \infty$ . Since E(D) is finite, d is required to be much less than N. Since the sample mean is an estimator for the mean of a Poisson distribution, and since D is approximately Poisson distributed, combining (i) and (ii) we obtain (4) and (5). If, in addition, all s classes are equally likely,  $C = n_d/s$ . Solving for s in (4) and (5) yields Corollary 3.

The role of the "low coverage" assumption in this paper is to compel a function of C, (ii), to converge in probability to a constant. It is important to recall that C is not a parameter of any distribution, but rather a random variable. Thus the estimation of C by a random variable has sources of error in each random variable. The restrictive assumptions reduce that to one source of error, which is handled by (i). Presumably the coverage of a moderate coverage sample could be made to conform to a normal limit law, but it is not clear how to do so. Normal limit laws were discussed further in Example 1.

PROOF OF THEOREM 2. The proof of Theorem 2 is similar to that of Theorem 1, but the differences are worth noting. In the context of Theorem 2,

$$E(D) = E(\sum D_i) = \sum P(X_i \ge 2) \sim \sum M_i (M_i - 1) p^2 (1 - p)^{M_i - 2} / 2$$
$$\sim \sum M_i (M_i - 1) p^2 / 2 \to m$$

by (9) and (10). Since the  $D_i$ 's are independent and  $P(D_i = 1) \to 0$  uniformly in i, D is asymptotically Poisson with mean m. This proves (i).

Since N is binomially distributed and  $E(N) = p \sum M_i \rightarrow \infty$ ,

$$(15) {N - E(N)}/E(N) \rightarrow_P 0.$$

Combining

(16) 
$$E(C-p)E(N)/2 \to m$$

and

(17) 
$$\operatorname{Var}\{(C-p)E(N)/2\} \to 0$$

yields

$$(18) (C-p)E(N)/2 \to_P m.$$

This and (15) yield

$$(19) (C-p)N/2 \to_P m.$$

This is (ii). To prove (16),

$$(C - p)E(N) = \{ (\sum M_i Y_i / \sum M_i) - p \} p \sum M_i = p \sum M_i Y_i - p^2 \sum M_i$$
  
=  $p \sum (M_i - 1) Y_i + p \sum Y_i - p^2 \sum M_i$ ,

and

$$E(p \sum Y_i - p^2 \sum M_i) \sim p \sum M_i p(1-p)^{M_i-1} - p^2 \sum M_i \rightarrow 0$$

and

$$E\{p \sum (M_i - 1)Y_i\} \sim \sum (M_i - 1)M_i p^2 (1 - p)^{M_i - 1} \rightarrow m.$$

To prove (17),

$$Var\{(C-p)E(N)\} = E^{2}(N)Var C \le p^{2}(\sum M_{i})^{2} \sum M_{i}^{2}(pM_{i})/(\sum M_{i})^{2}$$
  
 
$$\le p \max M_{i} \sum M_{i}^{2} p^{2} \to 0$$

By (9) and (10). Then (19) follows from (18) and (15) by adding and subtracting E(N). Suppose, for (iii), that  $M_i = M$  for all i. Then

$$E(N)E(C) \sim \sum M^2 p^2 = \{M/(M-1)\} \sum M(M-1)p^2 \to 2Mm/(M-1).$$

PROOF OF THEOREM 3. Note that the existence of  $E(M^3)$  implies the existence of  $E(M^2)$  and E(M). The first two conditions imply  $ps \to \infty$ , so (8) holds with probability 1. Because  $p^2s \to m' > 0$  and because  $E\{M(M-1)\}$  exists and is not zero, (10) is implied. To obtain (9), note first that

$$1 \ge P(p \max_{1 \le s} M_i < \varepsilon) = F^s(\varepsilon/p) = [1 - \{1 - F(\varepsilon/p)\}]^s \ge 1 - s(1 - F(\varepsilon/p)).$$

Since  $p^2s \to m'$ ,  $\varepsilon/p \sim \varepsilon' s^{1/2}$  and since  $s \to \infty$  we need only that  $x^2\{1 - F(\varepsilon'x)\} \to 0$ . Recall that if  $E(M^3)$  exists then  $\int x^2\{1 - F(x)\} dx$  exists, implying  $x^2\{1 - F(x)\} \to 0$ , which suffices for (9). Theorem 3 is proven.

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