Nonparametric Estimation of Species Richness

Eric P. Smith
Department of Statistics, Virginia Polytechnic Institute and State University,
Blacksburg, Virginia 24061, U.S.A.

and

Gerald van Belle
Department of Biostatistics, University of Washington, Seattle, Washington 98195, U.S.A.

SUMMARY

Two procedures, the jackknife and the bootstrap, are discussed as methods for estimating the number of species by the sampling of quadrats. Explicit formulas for both procedures are presented and evaluated under a model with a random distribution of individuals. The jackknife and bootstrap are shown to reduce the bias although they underestimate the actual number of species if there is a large number of rare species and the number of quadrats sampled is small. When a small number of quadrats is sampled, the jackknife is shown to give better estimates. When the number of quadrats is large, the jackknife tends to overestimate the number of species and the bootstrap performs better.

1. Introduction

In many biomonitoring studies, the response of communities of organisms to pollution is of interest. Often, data on the abundances of the organisms are summarized by an index, such as a diversity measure. Changes in the community are then associated with changes in the measure. Although the measures used to assess such changes are subject to criticism (Hendrickson, 1979; Hurlbert, 1971), this approach is commonly used.

One popular group of measures consists of measures based on the number of species in the community, for example species-richness measures (Sanders, 1968; Smith and Grasse, 1977). A problem that has received considerable attention is the sampling problem associated with estimating and testing the simplest species-richness measure, namely the number of species in the community (Sanders, 1968; Heck, van Belle and Simberloff, 1975). In comparing the number of species at two sites, Sanders (1968) observed that the number of species was dependent on the size of the sample, and suggested that the measures should be adjusted for sample-size bias by using simulation (the rarefaction method). Heck et al. (1975), using the work of Harris (1959), presented exact formulas for the adjustment, which are based on sampling individuals with or without replacement. However, there are two possible problems in the application of this approach. First, in many cases an experimenter samples area rather than individuals. In sampling benthic macroinvertebrates, for example, a sample may consist of a volume of soil taken with a core or grab device (Holme and McIntyre, 1971). Second, as noted by Heck et al. (1975), individuals are often highly clustered so random-sampling models do not strictly apply. Abundances of benthic species are often modelled with a negative binomial distribution (Downing, 1979; Resh, 1970). The estimates derived from multinomial models (e.g. sampling with replacement) are thus inappropriate and underestimate the actual variance (Kempton, 1977; Lyons and Hutcheson, 1978).

Key words: Quadrat sampling; Bootstrap; Jackknife.
Several authors, recognizing this problem, have suggested the jackknife method as an approach for estimating diversity measures and, in particular, the number of species when quadrat sampling is used (Zahl, 1977; Routledge, 1980; Heltshe and Forrester (1983). The jackknife method was introduced by Quenouille (1949) as a method for reducing bias. Tukey (1958) suggested that the technique could also be used to obtain approximate confidence intervals in situations where standard methods are difficult to apply. Conditions for the asymptotic normality and hence validity of the approximate confidence intervals have been presented by Arvesen (1969). A review and some applications were given by Miller (1974). For data based on quadrats, Zahl (1977) suggested treating each quadrat as a sample and then jackknifing the quadrats to estimate diversity. This approach was used by Heltshe and Forrester (1983) to estimate the number of species and to provide explicit estimates for the first-order jackknife estimate and an estimate of its variance.

In this paper, we describe, develop and compare two nonparametric methods for estimating the number of species under quadrat sampling, namely the jackknife method and the bootstrap method of Efron (1979). In §2, the two methods are described. In §3 we present estimators of the number of species for the two methods. To compare the methods, randomness models are used. Some possible models are considered in §4 and the estimators are evaluated under one of these models. Some advantages and disadvantages are discussed in §5. Formulas are given in reduced form, with more details presented by E. P. Smith and G. van Belle in an unpublished report (SIAM Institute for Mathematics and Society Technical Report No. 9 Biomathematics Group, University of Washington, 1982). Although the variances of the estimators are important, interest here lies primarily in the expectation of the estimators.

2. Estimation Procedures

The jackknife and the bootstrap methods assume that the quadrats are independent and represent a sample from the same distribution. No assumption, however, is made about the relationships among species within a quadrat.

2.1 Jackknife Method

Suppose one is interested in estimating some parameter, \( \theta \), using \( \hat{\theta} = f(x_1, x_2, x_3, \ldots, x_n) \), where \((x_1, x_2, \ldots, x_n)\) is a sample of \( n \) independent observations with cumulative distribution function \( F(\theta, X) \). Assume that \( \hat{\theta} \) is a reasonably good estimate of \( \theta \). To get the jackknife estimate, one performs the following sequence of steps:

(i) remove one of the observations, say, \( x_i \);
(ii) compute the estimate of \( \theta \) based on \((x_1, x_2, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n)\) and denote it by \( \hat{\theta}_{-i} \);
(iii) compute the pseudovalue \( \hat{\theta}_i = n\hat{\theta} - (n - 1)\hat{\theta}_{-i} \).

Steps (i) to (iii) are repeated \( n \) times for \( i = 1, \ldots, n \). The jackknife estimate \( J_n(\theta) \) is then given by

\[
J_n(\theta) = 1/n \sum\hat{\theta}_i.
\]

This estimate is known as the first-order jackknife and is useful for reducing bias of order \( 1/n \).

The estimate of the sampling variance of this estimate is given by

\[
\text{var}_{\text{est}}[J_n(\theta)] = \sum_{i=1}^{n} [J_n(\theta) - \hat{\theta}_i]^2/\{n(n - 1)\}.
\]
Schucany, Gray and Owen (1971) generalized the jackknife to remove higher-order bias by first removing one element at a time, then removing \((n/2)\) groups of size 2 and so on. If this is done for groups of up to size \(k\), the bias is removed to order \(O(1/n^2)\). The formula for the \(k\)th-order jackknife is

\[
J_k^*(\theta) = (k!)^{-1} \sum_{j=0}^{k} \frac{\hat{\theta}_{(j)}(-1)}{j} \binom{k}{j} (n-j)^k,
\]

where \(\hat{\theta}_{(j)}\) is the mean of the estimates based on removing groups of size \(j\). This formula is a reduction of Equation (2.7) given by Miller (1974).

2.2 Bootstrap Method

Efron (1979) developed the bootstrap as a method related to the jackknife but more widely applicable and dependable. Asymptotic properties of bootstrap estimates have been discussed by Singh (1981) and by Bickel and Freedman (1981). The bootstrap method typically requires simulation methods for estimation of the parameter and its variance.

Assume again that there are \(n\) iid observations from an unknown cumulative distribution function, \(F\). The bootstrap procedure (Efron, 1979) uses the following steps:

(i) construct the empirical probability distribution, \(F\), by putting mass \(1/n\) at each of the \(x_i\);
(ii) draw a sample of size \(n\) from the \(n\) data points with replacement; this constitutes the ‘bootstrap’ sample;
(iii) calculate the estimate of \(\theta\) based on the bootstrap sample;
(iv) repeat Steps (ii) and (iii) \(N\) times to get \(N\) estimates of \(\theta\), denoted \(\hat{\theta}_{(i)}\), \(i = 1, 2, \ldots, N\) (with \(50 < N < 200\)).

The bootstrap estimate, \(B_n(\theta)\), is then given by

\[
B_n(\theta) = (1/N) \sum_{i=1}^{N} \hat{\theta}_{(i)},
\]

with sampling variance

\[
\text{var}_{es}[B_n(\theta)] = (N - 1)^{-1} \sum_{i=1}^{N} [\hat{\theta}_{(i)} - B_n(\theta)]^2.
\]

3. Nonparametric Estimation of the Number of Species

In this section, exact expressions are presented for estimating the number, \(S\), of species by the jackknife and bootstrap methods. We extend to a \(k\)th-order jackknife some results already presented for the first-order jackknife by Heltshe and Forrester (1983).

3.1 Jackknife Estimate of \(S\)

The jackknife estimate is based on the number of species lost when quadrats are removed. If one quadrat, say Quadrat \(i\), is removed, the remaining number of species is

\[
\hat{S}_{-i} = S_0 - r_{1i},
\]

where \(r_{1i}\) is the number of species found only in Quadrat \(i\), and \(S_0 = \hat{S}\) is the observed number of species. If two quadrats are removed, say \(i\) and \(j\), the number of species in the sample is

\[
\hat{S}_{-ij} = S_0 - r_{1i} - r_{1j} - r_{1ij}.
\]
where $r_{ij}$ is the number of species found only in both Quadrats $i$ and $j$ and so on. To obtain the general jackknife estimate, (2.1) is used with $\hat{\theta}_{ij}$ denoting the mean of the estimates formed by removing a group of $j$ quadrats. An explicit expression for the $k$th-order jackknife is given by

$$J^*_1(S) = S_0 + \left(\sum_{j=1}^{k} r_{ij} \sum_{i=j}^{k} (-1)^{i+j} \binom{k}{i}(n-i)(n-j-1)/i\right)/k!,$$

where $r_{i(1)} = \sum_{j=1}^{n} r_{ij}$ is the number of species found in exactly one quadrat, $r_{i(2)} = \sum_{j<i} r_{ij}$ is the number of species found in exactly two quadrats, etc.

For $k = 1$, we have, from Heltshe and Forrester (1983), the estimate

$$J^*_1(S) = S_0 + [r_{i(1)}(n-1)]/n,$$

and for $k = 2$,

$$J^*_2(S) = S_0 + \left(\sum_{j=1}^{k} r_{ij} \sum_{i=j}^{k} (-1)^{i+j} \binom{k}{i}(n-i)(n-j-2)/i\right)/n(n-1).$$

Although some formulas will be presented for the general $k$th-order estimate, attention will be focused mainly on the first-order estimate.

The estimate of the variance for the first-order jackknife is

$$\text{var}_{\text{est}}(J^*_1(S)) = \frac{1}{n} \binom{\frac{1}{n}}{r_{i(1)}}^{2},$$

this may be written as

$$\text{var}_{\text{est}}(J^*_1(S)) = \frac{1}{n} \binom{\frac{1}{n}}{r_{i(1)}}^{2},$$

where $f_j$ is the number of quadrats with $j$ "unique" species (Heltshe and Forrester, 1983. Formulas for estimating the variance of the second-order jackknife have been given by Sharot (1976) and by Frangos (1980).

### 3.2 Bootstrap Estimate of $S$

The bootstrap estimate is formed by sampling $n$ quadrats from the $n$ samples for which there are data available. We are interested in estimating and adjusting for the bias, and also in estimating the variance. The approach to estimating the bias under sampling with replacement follows the methods of Harris (1959) and Sanders (1968).

Suppose we have a sample of size $n$ taken with replacement from the sample quadrats. Let $I_j = 1$ if Species $j$ is present in the bootstrap sample and let $I_j = 0$ if Species $j$ is absent. Let $S_0$ denote the number of species in the original sample and let $\hat{S}_0$ denote the number in the bootstrap sample, Then,

$$\hat{S}_0 = \sum_{j=1}^{S_0} I_j.$$

Under bootstrap sampling the expected value of $\hat{S}_0$ is given by

$$E_{\theta}(\hat{S}_0) = \sum_{j=1}^{S_0} E_{\theta}(I_j).$$

Now under sampling with replacement,

$$E_{\theta}(I_j) = pr_{\theta}(I_j = 1) = 1 - (1 - Y_{j//n})^n,$$
where $Y_{ij}$ is the number of quadrats in which Species $j$ is present. The estimate of the bias is then

$$\text{Bias}_{\text{est}}(\hat{S}_0) = \sum_{j=1}^{S_0} (1 - Y_{ij}/n)^n,$$

and the bootstrap estimate of $S$ is

$$B_d(S) = S_0 + \sum_{j=1}^{S_0} (1 - Y_{ij}/n)^n.$$

Note that $B_d(S)$ has a maximum value of

$$S_0 \left[ 1 + \left( \frac{n - 1}{n} \right)^n \right]$$

since $Y_{ij}$ is $\geq 1$. The smallest value of $B_d(S)$ is $S_0$ and is realized if and only if all species occur in all quadrats.

The estimate of the variance uses the same approach:

$$\text{var}_{\text{est}}(\hat{S}_0)$$

$$= \sum_{j=1}^{S_0} \left[ 1 - (1 - Y_{ij}/n)^n - (1 - Y_{ij}/n)^n \right]^2$$

$$+ \sum_{j\neq k} \sum_{i\neq j} \left[ 1 - (1 - Y_{ij}/n)^n - (1 - Y_{ik}/n)^n + (Z_{jk}/n)^n \right]$$

$$- \sum_{j\neq k} \sum_{i\neq j} \left[ (1 - Y_{ij}/n)^n + (1 - Y_{ik}/n)^n \right]$$

$$= \sum_{j=1}^{S_0} (1 - Y_{ij}/n)^n \left[ 1 - (1 - Y_{ij}/n)^n \right] + \sum_{j=1}^{S_0} \sum_{k \neq j} \left[ Z_{jk}/n^2 - (1 - Y_{ij}/n)^n(1 - Y_{ik}/n)^n \right],$$

where $Z_{jk}$ is the number of quadrats in which both Species $j$ and $k$ are jointly absent.

4. Evaluation under Randomness

4.1. Randomness Models

To evaluate the performance of the methods, the expectations of the estimates were computed under a random spatial distribution model. Several models are available for comparing estimators under the assumption of randomness. Although these models simplify the actual sampling, they provide a useful starting point for evaluating the properties of the estimators. As will be shown, one of the models is useful when individuals are not distributed randomly. Heck et al. (1975), in discussing the rarefaction method, suggested a multinomial sampling model. Suppose that a sample of $n$ individuals is taken from each quadrat. If the individuals are randomly distributed, then the vector of species counts, conditioned on $N$, is multinomial. For a single quadrat,

$$E(S_0) = S - \sum_{j=1}^{S} (1 - p_j)^n,$$

where $p_j$ is the proportion of Species $j$ in the total area. If $n$ quadrats are sampled,

$$E(S_0) = S - \sum (1 - p_j)^{nN}.$$

An alternative approach, proposed for analyzing species-area relationships, is the
'random placement' model due to Coleman (1981). Assume that a region with unit area is
divided into $m$ quadrats of equal area, so each quadrat has an area of size $a = 1/m$. Assume
that the number of individuals of Species $j$ is known to be $n_j$ ($j = 1, \ldots, S$). Then if
$n < m$ quadrats are sampled,

$$E(S_0) = S - \sum_{j=1}^{S} (1 - na)^{n_j}. \tag{4.1}$$

One problem with using this model is that the $n_j$ are assumed to be known. In a third
approach, which relaxes this assumption, it is assumed that the abundance of Species $j$
follows a Poisson distribution with mean abundance $\lambda_j$ over the area. The distribution in a
quadrat is Poisson with mean abundance $\lambda_j/m = \lambda_j a$. Then, setting $q_j = \exp(-\lambda_j/m),

$$E(S_0) = S - \sum_{j=1}^{S} q_j^{n_j}. \tag{4.1}$$

The three models are quite similar. Note that

$$q_j^{n_j} = \exp(-n\lambda_j/m) = (1 - p_j)^{n_j},$$

where

$$p_j = \lambda_j/\sum \lambda_j = (\lambda_j/m)/N.$$  

Additionally,

$$\exp(-n\lambda_j/m) = (1 - na)^{n_j},$$

where $a = 1/m$. Hence, the application of any of these three models should yield similar
results.

The Poisson model has an advantage over the others in that extensions are available for
nonrandom models. In most applications, organisms are not distributed randomly and the
Poisson model for the distribution of organisms is not applicable. Benthic insects, for
example, are almost always highly clustered. In these cases, experimenters often apply the
negative binomial model with parameters $K_j$ and $P_j$. It can be shown that the random
model may be used in the negative binomial case by taking $\lambda_j = K_j \ln(1 + P_j)$. If the negative
binomial model results from a clustering process, $\lambda_j$ is the mean number of clusters (see
Pielou, 1969, p. 84).

4.2 Expectation under Randomness

The estimators are compared first by computing their expectation under the Poisson model.
For the jackknife method,

$$E|J'_k(S)| = E(S_0) + \left\{ \sum_{j=1}^{k} E(r_{(j)}) \sum_{m=j}^{k} (-1)^{m-j} \binom{k}{m}(n - m)! \binom{n - j}{m - j} / m! \right\} / k!, \tag{4.2}$$

where $r_{(j)}$ is the number of species found only in $j$ quadrats. Now

$$E(r_{(j)}) = \sum_{i=1}^{S} \binom{n}{j} q_i^{n_j} (1 - q_i)^{n_j},$$

and $E(S_0)$ is given by (4.1). For $k = 1$, (4.2) reduces to

$$E|J'_1(S)| = S + \sum_{i=1}^{S} q_i^{n_j} (n - 1 - nq_i).$$
For the bootstrap estimate, we have
\[
E[B_n(S)] = E \left\{ S_0 + \sum_{j=1}^{S_n} (1 - Y_j/n)^\gamma \right\}.
\]
Now
\[
E \left\{ \sum_{j=1}^{S_n} (1 - Y_j/n)^\gamma \right\} = E \left\{ \sum_{j=1}^{S_n} I_j(1 - Y_j/n)^\gamma \right\}
= \sum_{j=1}^{S_n} \sum_{j=1}^{n} \binom{n}{y_j}(1 - y/n)^\gamma(1 - q_j)^\gamma q_j^{-y}.
\]
So,
\[
E[B_n(S)] = S - \sum_{i=1}^{S_n} \left[ q_i^n - \sum_{j=1}^{n} \binom{n}{y_j}(1 - y/n)^\gamma(1 - q_j)^\gamma q_j^{-y} \right].
\]
Under the randomness model,
\[q_i = \exp(-\lambda_i/m).\]
Note that the multinomial model could be applied by taking
\[q_i = (1 - p_i)^\gamma.\]

4.3 Evaluation and Comparison under Randomness

Under the Poisson model, one needs only to consider the effect of the density of one species, since the total effect is the sum of the parts, i.e. \(E(S_0) = \sum E(I_j).\) In Figs 1 and 2, the unadjusted bias is compared with the bias after adjustment for values of mean density \(\lambda_i/m\) by the jackknife and bootstrap methods. To indicate variability, error bars (± one standard deviation) have been drawn for the unadjusted estimator. The variance of the unadjusted estimator for one species is
\[\text{var}(I_i) = q_i^n(1 - q_i^n),\]
where \(q_i = \exp(-\lambda_i/m).\)

From the Figures, one observes that the jackknife-adjusted bias is always greater than the bootstrap-adjusted bias, which indicates that the jackknife compensates more for bias than the bootstrap. For both the estimators, there is a point at which the bias is adjusted to zero. As one would expect, the bias also tends to zero as the density increases. For densities near zero (rare species), the bias is not significantly reduced. For large densities, there is not much bias to reduce.

Note that for the jackknife estimate, the bias is zero if
\[q_i = (n - 1)/n.\]
A similar result holds for the bootstrap, although it is not possible to express it analytically.

In Table 1, explicit zero-bias values for several values of \(n,\) the number of quadrats sampled, are given for both the jackknife and bootstrap.

It is interesting that the maximum positive bias (overcompensation) changes only slightly for both procedures although the number of quadrats increases. For the jackknife method, the maximum positive bias occurs when
\[q_i = (n - 1)/(n + 1),\]
and its value is given by

$$\frac{(n - 1)}{(n + 1)}.$$  

As $n$ increases, this tends to $e^{-2} = .135$. In Table 1, we give some examples; note that the bootstrap follows a similar pattern, although the maximum bias is less.

One question that has received much attention in ecological studies is: ‘What area must be sampled in order to detect all species?’ (Kershaw, 1973). Often, an experimenter will sample quadrats sequentially, plot $S_0$ versus area sampled, and stop sampling when the graph of $S_0$ versus area becomes asymptotic. Figures 1 and 2 suggest an alternative approach. Since the bias of the unadjusted estimate is the probability of detecting a species minus 1, it is clear from the Figures that certain species have a very low probability of being sampled even if the number of quadrats is large. Hence, even if the species–area curve reaches an asymptote, one cannot be certain that all species will be in the sample. Using a nonparametric estimator, one can pick a density, say $\lambda^*$, and also the corresponding number of quadrats, such that the expected bias is always non-negative. This changes emphasis from minimum area to minimum density with non-negative expected bias. For example, suppose that the total area is divided into 100 quadrats. If we sample at least 10 quadrats we expect species with density greater than 10 per area (a density of .1 individual per quadrat) to be accounted for by the jackknife procedure, in the sense that the jackknife is approximately unbiased for that density. Note that the probability of observing a species with that density is .63.

While bias is determined by the rarity of species, the adjustment for bias depends on those species present in the sample. Consider the following two cases, and assume that the
Figure 2. Expected bias in the estimation of one species from 10 quadrats, versus density (individuals per quadrat): □ unadjusted bias, ○ jackknife bias, Δ bootstrap bias. Bars indicate plus or minus one standard deviation of the unadjusted estimator.

The jackknife method is used and \( n \) quadrats are sampled. In the first case, assume that in an area there are 20 species with densities below the density that yields zero bias for the jackknife. In the second case, assume there are 40 species, 20 with precisely the same densities as those in the first case, and 20 with densities above the density that yields zero bias for the jackknife. If \( n \) quadrats are sampled, the difference between the estimated number of species for the two cases will be at least 20. The 20 rare species will give precisely the same amount of negative bias in both cases. The 20 abundant species, however, have positive bias, and since bias is additive the number of abundant species will be estimated at more than 20 (see Fig. 1). The size of the difference between the estimated numbers of species depends on the closeness of the high densities to the density yielding maximum positive bias, and on the number of quadrats sampled.

A similar result also holds for the bootstrap procedure. Note that since the bias curve for the bootstrap always lies below that for the jackknife, the bootstrap will generally give a closer estimate if the number of quadrats is large. Otherwise, the jackknife will give more accurate results.

5. Discussion

One disadvantage in the use of nonparametric methods is that the estimates are bounded by \( 2S_0 \); hence they only work well if \( S_0 \) is sufficiently large or if the number of rare species is not too large relative to the total number of species. Other methods based on abundance models may be more useful when a small number of quadrats is used or if the number of rare species is large (see, for example, Efron and Thisted, 1976).
Table 1

Values of \( q_j \) and densities, \( \lambda_i/m \), yielding zero and maximum bias with the jackknife \((J)\) and the bootstrap \((B)\) methods

<table>
<thead>
<tr>
<th>( n )</th>
<th>( n )</th>
<th>( n )</th>
<th>( n )</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>10</td>
<td>15</td>
<td>20</td>
</tr>
<tr>
<td>( (J) )</td>
<td>( (B) )</td>
<td>( (J) )</td>
<td>( (B) )</td>
</tr>
<tr>
<td><strong>Zero bias</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( q_j )</td>
<td>.80</td>
<td>.67</td>
<td>.90</td>
</tr>
<tr>
<td>( \lambda_i/m )</td>
<td>.22</td>
<td>.41</td>
<td>.10</td>
</tr>
<tr>
<td><strong>Maximum bias</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( q_j )</td>
<td>.66</td>
<td>.52</td>
<td>.82</td>
</tr>
<tr>
<td>( \lambda_i/m )</td>
<td>.41</td>
<td>.66</td>
<td>.20</td>
</tr>
<tr>
<td>Bias</td>
<td>.131</td>
<td>.048</td>
<td>.134</td>
</tr>
</tbody>
</table>

The nonparametric methods have an advantage over the abundance-model approach in that one only needs presence-absence data rather than abundance data. Methods based on counting all individuals will be more expensive. Additionally, there may be problems in fitting the correct abundance model to the data, and large samples may be needed to estimate adequately the parameters of the abundance distribution. Slocomb and Dickson (1978) indicated that estimates of \( S \), based on simulated lognormal abundances, may vary tremendously. Lastly, the jackknife and bootstrap methods make no assumptions about the within-quadrat species interactions, whereas abundance models typically require an assumption of independence between species.

**ACKNOWLEDGEMENTS**

This research was funded by grants from the Alfred P. Sloan Foundation and the U.S. Environmental Protection Agency through SIMS (SIAM Institute for Mathematics and Society). Most of the work was done while the first author (E.P.S.) was at the University of Washington.

**REFERENCES**


Nonparametric Estimation of Species Richness


Received July 1982; revised January 1983