Estimating the Number of Species in a Population

by

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Abstract

This paper is concerned with the estimation of the number of species in a population. This is a familiar problem in ecological studies. Many scientists and statisticians have studied this problem. The method in estimating the number of species can be used in many other areas such as estimating the number of author’s vocabulary.

Many approaches have been proposed, some purely data-analytic and others based in sampling theory. We consider the latter case and focus on three methods in this paper. First one was based on the paper of Efron and Thisted [7]. Second one was given by Boneh, et. al. [4]. Third one was about Bayesian method and was proposed by Rodrigues, et. al. [22]. And we compare these methods using Mt. Kenya data and Mt. Mandalagan data.

As a result, the first two methods underestimate the number of species in the population for both data sets. The Bayesian method gives us more reasonable estimates and credible intervals. But we need to know the upper bound value beforehand, which is usually provided by an expert or analyst involved in the study. Thus, we need to construct another model which does not have to have the upper bound value for further research.
Acknowledgements

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Chapter 1

Background

1.1 Introduction

How many species are there? We may be interested in estimating the total number of species by considering the number of species obtained in a sample. For example, biologists and ecologists may be interested in estimating the number of species in a population of plants or animals (Mann)[16]. Numismatists may be concerned with estimating the number of dies used to produce an ancient coin issue (Stam)[25]. Linguists may be interested in estimating the size of an author’s vocabulary (Efron and Thisted)[7]. There are many other applications, including estimating the number of distinct records in a filing system where many records are duplicated (Arnold and Beaver)[1], undiscovered "observational phenomena" in astronomy (Harwit and Hildebrand)[14], errors in a software system (Bickel and Yahav)[3], executions in South Vietnam (Bickel and Yahav)[2], connected components in a graph (Frank)[10], and so on. And much previous work has stemmed from a parametric model due to Fisher, Corbet and Williams)[9], where Fisher fitted a theoretical distribution to Williams’s data on macrolepidoptera. Also, Good[11]
and, later, Good and Toulmin[12] derived a model based on a set of statistical hypotheses concerning the population frequencies of the individual species. However, throughout we focus exclusively on estimation of $C$ itself, we have to leave aside many interesting related topics, such as stochastic abundance models (Engen)[8], measurement of ”diversity” (Patil and Taillie)[19], and so on. We also avoid related areas such as capture-recapture problems (Pollock)[20] and estimation of the number of faults in software in continuous time, which, according to Nayak[18], ”can be regarded as a continuous analogue of the problem of estimating the number of species in a biological population.”

To estimate the number of species $C$ in a population, we take a sample of size $n$ from a population, finite or infinite, partitioned into $C$ classes, where $C$ is unknown. The outcome of this sampling theoretically can be represented by the random vector $\mathbf{n} = [n_1, \ldots, n_C]^\prime$, where $n_i$ is the number of sample items from the $i$th class, $i = 1, \ldots, C$ and $n_i > 0$. In short, the random vector $\mathbf{n}$ is not observable. Instead the observable random vector is $\mathbf{c} = [c_1, \ldots, c_n]^\prime$, where $c_j$ is the number of classes represented $j$ times in the sample, $j = 1, \ldots, n$. The problem is to estimate the number of classes $C$ based solely on the vector of frequencies of observed classes $c$. This vector $c$ is also called the ”frequencies of frequencies.” Herein $c$ will denote the total number of classes in the sample, so that $c = \sum_{j=1}^{n} c_j$. Note that

$$n = \sum_{i=1}^{C} n_i = \sum_{j=1}^{n} j c_j.$$  

We prefer to write the total number of observed individuals $n$ as the second sum because the number of species in the population $C$ is unknown.

Many approaches have been considered. Some of them are based on data-analytic methods and others are based on sampling-theoretic methods (see Figure 1.1). In
this paper, we focus on the latter case. If a population is finite, samples may be taken with replacement (multinomial sampling) or without replacement (hypergeometric sampling), or by Bernoulli sampling. But a finite population will not be realistic in many situations because the population size will be unknown. If a population is infinite, samples may be taken by multinomial sampling or Bernoulli sampling, or the samples may be the result of random Poisson contributions of each class. Given a sampling model, one may approach estimation of the number of species via a parametric or nonparametric formulation; in either case there may be frequentist and Bayesian procedures.
Figure 1.1: Existing Literature on the Problem of Estimating the Number of Classes in a Population
1.2 Statement of the Problem

This project aims to achieve the following:

First of all, we give a comprehensive review of methods or approaches to the problem of estimating the number of species in a population. Secondly, we examine in detail the different models used in Bayesian approaches. Lastly, we propose a simple Bayesian model in estimating the number of species in a population.

On two datasets of the number of species in a natural population, we employ methods from Efron and Thisted [7] and Boneh, Boneh and Caron [4] as implemented in [21] and the Bayesian procedure.

The first dataset is the species distribution of a sample from Mount Kenya. This dataset was used by Lewins and Joanes [15]. An experiment was performed to get information on the insect population within a particular region. In consultation with the experimenters an appropriate prior mode of 45 species was identified. And also the experimenters were confident that the total number of species in the population lay between 35 and 55. The dataset is shown in Table 1.1. Here, the sample size, $n$, is 1043 and the total number of observed species in the sample, $s'$, is 32.

The second dataset is the species distribution of a sample from Mount Mandalagan. This dataset was used by Cordon [6]. He obtained these data through counting the number of different kinds of trees in one hectare plot with a dimension of 500m $\times$ 20m. In this case, the unseen species is the unobserved species of trees in one hectare plot that exist in Mt. Mandalagan. The data set is shown in Table 1.2. Here, the sample size is 582 in one hectare plot and there are 49 distinct species of trees in the area.
Table 1.1: Number of Observed Species of Insects in the Sample in Mt. Kenya

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<td><strong>Total</strong></td>
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Table 1.2: Number of Observed Species of Trees in One Hectare Plot in Mt. Mandalagan, Negros Occidental

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Chapter 2

Review of Related Literature

In this chapter, the papers most relevant to this research is discussed. Comments about the features of previous research are also given.

2.1 Estimating the Number of Species: A Review by J. Bunge and M. Fitzpatrick [5]

This paper, to date, has given the most comprehensive review of the available methods and approaches to estimating the number of species in a population. The authors give a very detailed and structured presentation of the problem and approaches to it. Some of the details we give below.

Suppose that a population, finite or infinite, is partitioned into \( C \) classes. In many cases we are interested in estimation of \( C \) itself. Although estimation of the relative class proportions is well understood when \( C \) is known, estimation of \( C \) itself appears to be quite difficult. Unfortunately, many interesting related topics are excluded from this paper. Given a sampling model, one may approach estimation of \( C \) via a parametric or nonparametric formulation; in either case there may be
2.1.1 Finite Population, Hypergeometric Sample

Suppose the population is finite with known size $N$. Let $N_i$ denote the number of units in the $i$th class, $i = 1, ..., C$, $\sum_{i=1}^{C} N_i = N$, and let $M = \max_{1 \leq i \leq C} N_i$. If $n$ items are sampled at random without replacement from this population, then the random vector $\mathbf{n}$ has a multiple hypergeometric distribution with probability mass function (pmf) $P_n(\mathbf{n}) = \binom{N}{n} \times \prod_{i=1}^{C} \binom{N_i}{n_i}$. The pmf of the observable random vector $\mathbf{c}$, $p_c(\mathbf{c})$, is simply $p_n(\mathbf{n})$ summed over all points $\mathbf{n}$ corresponding to $\mathbf{c}$: $p_c(\mathbf{c}) = \sum_{S} p_n(\mathbf{n})$, where $S = \{n; \# \{n_i = j\} = c_j, j = 1, ..., n\}$. For this model Goodman (1949) showed that if $n \geq M$, there is a unique unbiased estimator of $C$. The estimator is

$$\hat{C}_{GOODMAN1} = c + \sum_{j=1}^{n} (-1)^{j+1} \frac{(N - n + j - 1)! (n - j)!}{(N - n - 1)! n!} c_j.$$ 

Unfortunately, although this estimator is an uniformly minimum variance unbiased (UMVU), its variance is so large in many cases. And it needs not even be positive.

In contrast, Shlosser (1981) took an asymptotic approach in which $N, n \to \infty$ in such a way that $n/N \to q \in (0, 1)$. On this basis, he derived an estimator which is always greater than equal $c$. The estimator is

$$\hat{C}_{SHLOSSER} = c + c_1 \left( \sum_{i=1}^{n} i q (1 - q)^{i-1} c_i \right)^{-1} \sum_{i=1}^{n} (1 - q)^i c_i.$$ 

The estimator performed reasonably well in his simulations for sampling fractions as low as 10%. But a problem here is that Shlosser did not calculate the bias or variance of this estimator. However, this estimator is much better than the one
derived by Goodman.

2.1.2 Finite Population, Bernoulli Sample

Suppose that the \( N \) items of the population enter the sample independently, each with probability \( p \). Then the total sample size is a binomial \((N, p)\) random variable, the \( i \)th class independently contributes a binomial \((N_i, p)\) random number of items to the sample, and \( p_n(n) = p^n (1 - p)^{N - n} \prod_{j=1}^{C} \binom{N_i}{n_i}, \sum_{i=1}^{C} n_i = n \), but \( p_c(c) = \sum_{S} p_n(n) \). Goodman (1949) considered such Bernoulli sampling for known \( p \) and derived the unbiased estimator. The estimator is

\[
\hat{C}_{GOODMAN2} = c + \sum_{j=1}^{n} (-1)^{j+1} \left( \frac{1 - p}{p} \right)^{j} c_j.
\]

The undesirable properties of \( \hat{C}_{GOODMAN1} \) are shared by \( \hat{C}_{GOODMAN2} \). This equiprobable case, the same probability \( p \), will not be realistic, so different \( p_i \)'s will be more realistic.

2.1.3 Infinite Population, Multinomial Sample

Suppose that we take a sample of size \( n \) at random from an infinite population partitioned into \( C \) classes in proportions \( \pi = [\pi_1, ..., \pi_C] \), \( \sum_{j=1}^{C} \pi_i = 1 \). In the infinite population case, \( n \) has a \( C \)-dimensional multinomial distribution, with pmf

\[
p_n(n) = \binom{n}{n_1, ..., n_C} \times \prod_{i=1}^{C} \pi_i^{n_i}, \sum_{i=1}^{C} n_i = n.
\]
2.2 Bayesian Estimation of the Number of Species

by W. A. Lewins and D. N. Joanes [15]

In this paper, a Bayesian approach is used to estimate the number of species in a population. Many works have been done by Fisher, Corbet and Williams (1943), and Good and Toulmin (1956). But the estimation of the total number of species in the population was not the prime concern of those works. When such estimation has been the main aim, it has usually been assumed that the species have equal relative abundances. More recently, nonequiprobable models have been derived by Efron and Thisted (1976) and Hill (1979). Hill’s model is based on a zero-truncated negative binomial prior distribution for the number of species, and results of this paper are also based on this distribution.

2.2.1 Model of W. A. Lewins and D. N. Joanes

Let \( s \) be the number of species in a population of infinite size, and consider a sample of size \( n \) containing \( s' \) species (\( n << \) population size). Let \( P_i(i = 1, ..., s) \) denote the species relative abundances in the population with \( \sum_{i=1}^{s} p_i = 1 \). We may write the joint prior distribution for \( s, p_1, ..., p_s \), for a given prior parameter \( k \), as

\[
P(s) f(p_1, ..., p_s|s, k) = \frac{\Gamma(k s)}{\Gamma(k)} \prod_{j=1}^{s} p_j^{k-1}.
\]

By the conventional Bayesian approach, we may write the posterior distribution for \( s \) as

\[
P(s|data, k) \propto \int ... \int P(s) f(p_1, ..., p_s|s, k) P(data|p_1, ..., p_s, s, k) dp_1 ... dp_s,
\]
where \( P(data|p_1, ..., p_s, s, k) \) is the likelihood function. We assume that the species appearing in the sample are not distinguishable. Thus, the likelihood function is the sum of several multinomial terms.

Hence, by means of the nonsymmetric Dirichlet integral, the posterior distribution of \( s \) can be evaluated as

\[
P(s|data, k) \propto P(s) \left\{ \frac{B(n, ks)}{B(s', s - s' + 1)} \right\}, s \geq s',
\]

where the standard beta function \( B(x, y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x + y)} \).

Taking \( P(s) \) to be the zero-truncated negative binomial distribution

\[
P(s) = \binom{s + r - 1}{s} \left\{ \frac{\alpha^r(1 - \alpha)^s}{1 - \alpha^r} \right\}, 0 < \alpha < 1, s \geq 1,
\]

we obtain the posterior distribution

\[
P(s|data, k) \propto (1 - \alpha)^s \binom{s + r - 1}{s} \binom{s}{s'} \binom{ks + n - 1}{n}^{-1}.
\]

### 2.3 Estimating the Total Number of Distinct Species Using Presence and Absence Data by S. A. Mingoti and G. Meeden [17]

In this paper, they talk about the problem of estimating the total number of distinct species \( S \) in some specified region of investigation. If the elements in the region are discrete and countable, a random sample of individuals could be taken. Since this sampling procedure is difficult to implement in practice, quadrat sampling
is used here. This procedure is more feasible for many real situations. There are two
different ways to perform the quadrat sampling. One is that the region is divided
into $N$ quadrats of equal area, $N < \infty$, and then we take a random sample of $n$
quadrats from $N$, $n \geq 1$ and $n < N$. The other is to place at random $n$ quadrats
of equal area and fixed shape in the region of investigation. In both cases the $n$
quadrats in the sample are assumed to be disjoint and are totally observed. So if
quadrat sampling is performed in fact, a random sample of space is taken instead of
a random sample of individuals. Within each sampled quadrat the distinct species
present are observed and an empirical Bayes estimator of the total number of species
$S$ in the region is constructed. Finally, they develop an approximate estimate of
standard deviation for the empirical Bayes estimator and study the behavior of
certainty intervals based on this estimate.

2.3.1 Model of S. A. Mingoti and G. Meeden

Suppose that the region of investigation is divided into $N$ disjoint quadrats of
equal area, not necessarily of the same shape, $N < \infty$. Let $S$ be the total number of
distinct species present in the region and let $s_1, \ldots, s_S$ be the names of those $S$ species.
$s_1, \ldots, s_S$ are unknown and $S$ is assumed to be finite. Let $p_i$ be the probability of
species $s_i$ being observed in a typical quadrat of the region, $i = 1, \ldots, S$. $p_i$ is not
necessarily the probability that the species $s_i$ is present in the quadrat but can also
be the probability of observing the species $s_i$ in the quadrat.

Let’s assume that $p_1, \ldots, p_S$ are independent and identically distributed random
variables from a beta density with parameters $\alpha > 0$ and $\beta > 0$, $\alpha$ and $\beta$ being
known. Suppose a random sample of $n$ quadrats, $n \geq 1$, is taken from the collection
of $N$ quadrats. Let $X_i$ be the number of quadrats in the sample where the species
$s_i$ was observed, $i = 1, \ldots, S$, and let $n_x$ be the number of species observed in exactly
\( x \) quadrats in the sample, \( n_x \in \{0, 1, \ldots, S\} \), \( x \in \{0, 1, \ldots, n\} \). Then for each species \( s_i \) the probability that it will be observed in exactly \( x \) quadrats in the sample is

\[
\gamma_x = \int_0^1 P(r(X_i = x|p_i)) \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} p_i^{\alpha-1}(1 - p_i)^{\beta-1} dp_i
\]

\[
= \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \int_0^1 \binom{n}{x} p^{x+\alpha-1}(1 - p)^{n-x+\beta-1} dp
\]

\[
= \binom{n}{x} \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \frac{\Gamma(x + \alpha)\Gamma(n + \beta - x)}{\Gamma(n + \alpha + \beta)}.
\]

So \( \gamma_x \) is the same for any species \( s_i \), and represents the probability that a typical species will be observed in exactly \( x \) quadrats of those \( n \) quadrats in the sample. Given \( S \) and \( \gamma_x (x = 0, 1, \ldots, n) \), \( n_x \) is a binomial random variable with expectation given by

\[
n_x = E_S(n_x) = S\gamma_x.
\]

### 2.4 The Relation Between the Number of Species and the Number of Individuals in a Random Sample of an Animal Population by R. A. Fisher [9]

He talks about the relationship between the Poisson Series and the Negative Binomial distribution first. If successive independent equal samples are taken from homogeneous material in biological sampling, the number of individuals observed in different samples will vary in a definite manner. The distribution of the number
observed will be the Poisson series, which has a single parameter \( m \) expressed in terms of the number expected. The distribution is given by

\[
e^{-m} \frac{m^n}{n!},
\]

where \( n \) is the variate representing the number observed in any sample and \( m \) is the number expected, which is the average value of \( n \). \( m \) will be proportional to the size of the sample taken.

An important extension of the Poisson series is provided by the supposition that the values of \( m \) are distributed in a known and simple manner. Since \( m \) must be positive, the simplest supposition as to its distribution is that it has the Eulerian form such that the element of frequency or probability with which it falls in any infinitesimal range \( dm \) is

\[
df = \frac{1}{(k-1)!} p^{-k} m^{k-1} e^{-m/p} dm.
\]

If we multiply this expression by the probability of observing \( n \) organisms and integrate with respect to \( m \) over its whole range from 0 to \( \infty \), we have

\[
\int_0^\infty \frac{1}{(k-1)!} p^{-k} m^{k-1} e^{-m/p} \frac{m^n}{n!} dm = \frac{(k+n-1)!}{(k-1)!n!} \frac{p^n}{(1+p)^{k+n}} \cdots \otimes,
\]

which is the probability of observing the number \( n \). Since this distribution is related to the negative binomial expansion

\[
\left(1 - \frac{p}{1+p}\right)^{-k} = \sum_{n=0}^{\infty} \frac{(k+n-1)!}{(k-1)!n!} \left(\frac{p}{1+p}\right)^n,
\]

it has become the Negative Binomial distribution. The parameter \( p \) is proportional.

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to the sample size and the parameter $k$ measures the variability of the different
expectations of the component Poisson series. The expectation, or mean value of $n$, is $pk$.

Next, he talks about the limiting form of the negative binomial, excluding zero
observations. In many of its applications the number $n$ observed in any sample may
have all integral values including zero. However, in its application to the number
of representatives of different species obtained in a collection, only frequencies of
numbers greater than zero will be observable, since by itself the collection gives no
indication of the number of species which are not found in it. Now, the abundance
in nature of different species of the same group generally varies very greatly, so that,
the negative binomial has a value of $k$ so small as to be almost indeterminate in
magnitude or indistinguishable from zero. That it is not really zero for collections
of wild species follows from the fact that the total number of species, and therefore
the total number not included in the collection, is really finite. However, the real
situation in which many species are so rare that their chance of inclusion is small is
well represented by the limiting form taken by the negative binomial distribution,
when $k$ tends to zero.

If we put $k = 0$ in right-hand side of expression $\otimes$, write $x$ for $p/(p + 1)$, so
that $x$ stands for a positive number less than 1, and replace the constant factor
$(k - 1)!$ in denominator by a new constant factor alpha in the numerator, we have
an expression for the expected number of species with $n$ individuals, where $n$ cannot
be zero,

$$\frac{\alpha}{n}x^n.$$
The total number of species expected is

\[ S = \sum_{n=1}^{\infty} \frac{\alpha}{n} x^n = -\alpha \log(1 - x). \]

The total number of individuals expected is

\[ N = \sum_{n=1}^{\infty} \alpha x^n = \frac{\alpha x}{1 - x}. \]

If \( x \) is eliminated from the two equations, it appears that

\[ S = \alpha \log \left(1 + \frac{N}{\alpha}\right), \quad N = \alpha (e^{S/\alpha} - 1), \]

and

\[ \frac{N}{S} = (e^{S/\alpha} - 1) \div S/\alpha. \]

These numerical processes are exhibited for fitting the series to observations containing given numbers of species and individuals, and for estimating the parameter \( \alpha \) representing the richness in species of the material sampled; secondly, for calculating the standard error of \( \alpha \), and thirdly, for testing whether the series exhibits a significant deviation from the limiting form used.
2.5 Estimating the Prediction Function and the Number of Unseen Species in Sampling with Replacement by S. Boneh, A. Boneh and R. J. Caron [4]

We introduce the two basic models presented by Boneh, Boneh and Caron which will be used as basis for the two estimators. Suppose there are $s$ species sampled independently with replacement and each has probabilities $p_1, ..., p_s$, $0 < p_i < 1$ so that $\sum_{i=1}^{s} p_i = 1$. Alternatively, consider $s$ parallel independent Poisson processes with positive parameters $\lambda_1, ..., \lambda_s$. The probabilities and the mean of the Poisson processes can be related by interpreting the occurrences of the $j$th Poisson process as observations of the $j$th species, with the parameters related by $p_j = \lambda_j / (\lambda_1 + ... + \lambda_s)$, $j = 1, 2, ..., s$.

Let $[−1, 0]$ be the time interval over which the occurrences of the Poisson processes were recorded. This time interval would correspond to a given information about a sample. A process is said to have been detected if there was at least one occurrence of that process. Let $D(t)$ be the number of new detections in $(0, t]$ but not in $[−1, 0]$. Its expected value, denoted by $\Psi(t) = E[D(t)]$, is called the prediction function. Let $N_k$ be the number of species observed exactly $k$ times in $[−1, 0]$, $k = 1, 2, ....$

We define and specify the prediction function $\Psi(t)$ as

$$\Psi(t) = \sum_{j=1}^{s} e^{-\lambda_j} - \sum_{j=1}^{s} e^{-\lambda_j(1+t)} = \sum_{k=1}^{\infty} (-1)^{k+1} E(N_k) t^k.$$
This prediction function computes the expected number of newly detected species in \((0, t]\) but not in \([-1, 0]\).

The three properties of the prediction function \(\Psi(t)\) are the following:

1. \(\Psi(t) = 0\)

2. \(\Psi(t)\) has a horizontal asymptote (i.e., \(\Psi(\infty) < \infty\))

3. \(\Psi(t)\) has infinite order alternating copositivity.

Boneh, Boneh and Caron suggest an alternative by expressing the prediction function, \(\Psi(t) = \sum_{j=1}^{s} e^{-\lambda_j} - \sum_{j=1}^{s} e^{-\lambda_j(1+t)}\), and then estimating the parameter \(s\) and \(\lambda_1, \ldots, \lambda_s\), rather than \(E(N_k)\). So, we get the maximum likelihood estimators (MLEs) for these parameters. In getting the MLE of \(s\), we consider all the number of distinct species according to the number of times that they appeared denoted by \(N_k\). Recall that \(N_k\) is the number of species that appeared \(k\) times. To maximize the value of \(s\), we get the total number of distinct species as will be given by \(N_k\) up to the maximum value of \(k\). Thus,

\[
\hat{s} = \sum_{k=1}^{k_{\text{max}}} N_k, 
\]

where \(k_{\text{max}} = \max \{k : N_k > 0\}\).

We have \(\hat{\lambda}_j, \ldots, \hat{\lambda}_{\hat{s}}\) for the MLEs of \(\lambda_1, \ldots, \lambda_s\), where \(\hat{\lambda}_j\) is the number of occurrences of the \(j\)th process during the interval \([-1, 0]\). Thus, an estimate of \(\Psi(t)\) is

\[
\hat{\Psi}(t) = \sum_{j=1}^{\hat{s}} e^{-\hat{\lambda}_j} - \sum_{j=1}^{\hat{s}} e^{-\hat{\lambda}_j(1+t)}
\]

Since processes can be observed with the same number of times \(N_k\), it will have
the same estimate for \( \hat{\lambda} \) so that these processes can be grouped. Hence,

\[
\hat{\Psi}(t) = \sum_{k=1}^{k_{\text{max}}} N_k e^{-k} - \sum_{k=1}^{k_{\text{max}}} N_k e^{-k(1+t)}
\]

This estimator is biased. In order to reduce the bias, Boneh, Boneh and Caron suggested a bias reduction algorithm given below.

Given \( N_k, k = 1, 2, ... \)

1. Calculate \( U_0 = \sum_{k=1}^{k_{\text{max}}} N_k e^{-k} \).

2. Set \( i = 1 \).

3. If \( U_0 \geq N_1 \), then set \( U_i = 0 \).

4. Set \( U_i = U_0 + U_{i-1} e^{-N_1/U_{i-1}} \).

5. If a stopping criterion is not met, replace \( i \) with \( i + 1 \) and repeat step 4.

A common stopping criterion for step 5 is to stop as soon as \( U_{i+1} - U_i < \delta \) for some predetermined \( \delta > 0 \) where \( \delta \) is a relatively small value. This means that if there is a very little difference between succeeding values \( U_i \) and \( U_{i+1} \) then the algorithm should be terminated.

Hence, the second estimator of the prediction function for estimating the number of unseen species, denoted by \( \hat{\Psi}^*(t) \), is given by

\[
\hat{\Psi}^*(t) = \hat{\Psi}(t) + U e^{-\hat{\lambda}^*} + U e^{-\hat{\lambda}^*(1+t)},
\]

where \( \hat{\Psi}(t) = \sum_{k=1}^{k_{\text{max}}} N_k e^{-k} - \sum_{k=1}^{k_{\text{max}}} N_k e^{-k(1+t)} \), \( U \) is the last iteration value, and \( \hat{\lambda}^* = N_1/U \).
2.6 Estimating the Number of Unseen Species: How Many Words Did Shakespeare Know? 
by B. Efron and R. Thisted [7]

We present the species trapping terminology of Efron and Thisted [7] that will be used in estimating the number of unseen species. Suppose there is a population consisting of \( S \) species where \( S \) is unknown. Suppose in a trapping procedure for one unit of time, we were able to sample \( s \) species where \( s = 1, 2, ..., S \). Let \( x_s \) be the random variable that represents the number of captured members of species \( s \). We only observe values of \( x_s \) which are greater than zero because there is no such thing as a negative number of species. The case \( x_s = 0 \) is negligible since it will not be counted in the sample. Moreover, we cannot possibly count the number of captured members of species \( s \) if we have no knowledge that this particular species \( s \) exists.

The basic distributional assumption for this trapping procedure is that members of species \( s \) enter the trap following a Poisson process. This means that members of species \( s \) enter the trap (success) per unit time. It is also assumed that the members of species \( s \) that enters the trap following a Poisson process has an expectation of \( \lambda_s \) per unit time. Thus, \( x_s \) has a Poisson distribution with mean \( \lambda_s, s = 1, 2, ..., S \).

We further assume that the individual Poisson processes are independent of one another.

The trapping period can be presented in the period \([-1, 0]\). Since we want to estimate the exact number of species in the sample, we wish to extrapolate from the counts in \([-1, 0]\) to a time \( t \) in the future. Extrapolating is similar to forecasting or predicting the future observations using observations from periods -1 to 0 to predict the observations for the next \( t \) periods, that is, period \((0, t]\). Recall that \( x_s \) denotes
the number of captured members of species \( s \) in time period \([-1, 0]\). This \( x_s \) will be helpful in knowing how many members of species \( s \) will be on the time period \((0, t]\). Let \( n_x \) be the number of species observed exactly \( x \) times in \([-1, 0]\). This value may be computed from the available values of \( x_s \). It will also be used, like \( x_s \), in computing the estimate for the unseen species. We present the estimator proposed by Efron and Thisted for the number of unknown species. Let \( \Delta(t) \) be the expected number of species observed in the period \((0, t]\) (future), but not in \([-1, 0]\) (observed period), or it is the expected number of new species to be found in the next \( t \) time units. Recall that \( \Psi(t) \) is the expected value of \( D(t) \), the number of new detections in \((0, t]\) but not in \([-1, 0]\). Thus, \( \Delta(t) \) is the same as \( \Psi(t) \).

\[
\Delta(t) = \Psi(t) = \sum_{j=1}^{x} e^{-\lambda_j} (1 - e^{-\lambda_j t}).
\]

Let \( n_x \) be the number of species observed exactly \( x \) times in \([-1, 0]\) which is similar to \( N_k \) based in our basic model. The expected value of \( n_x \) is denoted by \( \eta_x \). So, we have

\[
\Delta(t) = \Psi(t) = \sum_{k=1}^{\infty} (-1)^{k+1} E(n_k) t^k = \eta_1 t - \eta_2 t^2 + \eta_3 t^3 - \cdots.
\]

The right hand side of the equation above need not converge, but if we assume that it does, the equation below suggests the unbiased estimator for \( \Delta(t) \). The unbiased estimator of \( \Delta(t) \) is the first proposed estimator that will be used in estimating the number of unseen species. This is given by

\[
\hat{\Delta}(t) = n_1 t - n_2 t^2 + n_3 t^3 - \cdots.
\]

This equation, unfortunately, is useless for \( t \) larger than one because the geomet-
rically increasing magnitude of \( t^x \) produces wild oscillations as the number of terms increases. This then forces the series not to converge.

These methods described in the last two sections will be used in the numerical examples in Chapter 4.
Chapter 3

Bayesian Approach

3.1 Bayesian Inference

Bayesian statistical conclusions about a parameter $\theta$ is made in terms of a probability statement. This probability statement is conditional on the observed value of $y$, and in our notation is written simply as $p(\theta|y)$. In this section, we present the basic mathematics and notation of Bayesian inference.

3.1.1 Bayes’ Rule

In order to make probability statement about $\theta$ given $y$, we must begin with a model providing a joint probability distribution for $\theta$ and $y$. The joint probability mass or density function can be written as a product of two densities that are often referred to as the prior distribution $p(\theta)$ and the data distribution $p(y|\theta)$ respectively:

$$p(\theta, y) = p(\theta)p(y|\theta).$$
Simply conditioning on the known value of the data $y$, using the basic property of conditional probability known as Bayes’ rule, yields the posterior density:

$$p(\theta|y) = \frac{p(\theta, y)}{p(y)} = \frac{p(\theta)p(y|\theta)}{p(y)},$$

where $p(y) = \sum_{\theta} p(\theta)p(y|\theta)$, and the sum is over all possible values of $\theta$ (or $p(y) = \int p(\theta)p(y|\theta)d\theta$ in the case of continuous $\theta$). An equivalent form of the posterior density above omits the factor $p(y)$, which does not depend on $\theta$ and, with fixed $y$, can thus be considered a constant, yielding the unnormalized posterior density, which is the right side of the following expression:

$$p(\theta|y) \propto p(\theta)p(y|\theta).$$

These simple expressions encapsulate the technical core of Bayesian inference: the primary task of any specific application is to develop the model $p(\theta, y)$ and perform the necessary computations to summarize $p(\theta|y)$ in appropriate ways.

### 3.1.2 Prediction

To make inferences about an unknown observable, often called predictive inferences, we follow a similar logic. Before the data $y$ are considered, the distribution of the unknown but observable $y$ is

$$p(y) = \int p(y, \theta)d\theta = \int p(\theta)p(y|\theta)d\theta.$$  

This is often called the marginal distribution of $y$, but a more informative name is the prior predictive distribution: prior because it is not conditional on a previous observation of the process, and predictive because it is the distribution for a quantity
that is observable.

3.1.3 Likelihood

Using Bayes’ rule with a chosen probability model means that the data \( y \) affect the posterior inference, which is given by \( p(\theta) \propto p(\theta)p(y|\theta) \), only through the function \( p(y|\theta) \), which, when regarded as a function of \( \theta \), for fixed \( y \), is called the likelihood function. In this way Bayesian inference obeys what is sometimes called the likelihood principle, which states that for a given sample of data, any two probability models \( p(y|\theta) \) that have the same likelihood function yield the same inference for \( \theta \).

The likelihood principle is reasonable, but only within the framework of the model or family of models adopted for a particular analysis. In practice, one can rarely be confident that the chosen model is the correct model.

3.2 Hierarchical Bayesian Analysis for the Number of Species by J. Rodrigues, L. A. Milan and J.G. Leite [22]

We present a method for estimation of the number of species in a population through a hierarchical Bayesian model. Suppose \( X_i \) is the number of individuals from species \( i \) in the sample, \( i = 1, ..., N \); \( N \) is the number of species in the population; \( N_j = \sum_{i=1}^N I(X_i=j), j \geq 1 \) are the frequencies of frequencies where \( I_A \) means the indicator function of the set \( A \); \( n = \sum_{j \geq 1} jN_j \) is the sample size and \( W = \sum_{j \geq 1} N_j \) is the number of different species in the sample. This hierarchical Bayesian model was presented in [22] and we modify one step in generating samples from the conditional
posterior of one of the parameters.

We consider the situation where the random variables \((X_i, \theta_i), i = 1, \ldots, N\) are independent and \(N\) is given. The probability density of \(X_i\), given \(N\) and \(\theta_i\), is Poisson with the parameter \(\theta_i\), i.e.,

\[X_i|\theta_i, N \sim \text{Poisson}(\theta_i),\]

for \(i = 1, \ldots, N\). The likelihood function, \(L(N, \theta)\), is given by

\[L(N, \theta) = Pr [N_1 = n_1, N_2 = n_2, \ldots|\theta, N] = \sum_{x \in A} \prod_{i=1}^{N} \frac{\theta_i^{x_i} e^{-\theta_i}}{x_i!},\]

where \(N \geq w = \sum_{j \geq 1} n_j, \theta = (\theta_1, \ldots, \theta_N)\)
and \(A = \{x = (x_1, x_2, \ldots, x_N) : \sum_{i=1}^{N} I_{(j)}(x_i) = n_j, j = 1, 2, \ldots\}\).

Suppose each \(\theta_i\) has an independent prior density \(\pi(\theta|\lambda)\). For a given \(N\), the \(\pi\)-mixture distribution is

\[p_{\lambda}(j) = \int_{0}^{\infty} \frac{\theta^j e^{-\theta}}{j!} \pi(\theta|\lambda) d\theta.\]

We integrated the likelihood function above to eliminate the nuisance parameters \(\theta_i, i = 1, \ldots, N\), then we get

\[L_M(N, \lambda) = \frac{N!}{(N-w)!}\left(p_{\lambda}(0)\right)^{N-w} \prod_{j \geq 1} \left(\frac{p_{\lambda}(j)}{n_j!}\right)^{n_j} \prod_{j \geq 1} \left(\frac{p_{\lambda}(j)}{1 - p_{\lambda}(0)}\right)^{n_j} \prod_{j \geq 1} \left(\frac{p_{\lambda}(j)}{1 - p_{\lambda}(0)}\right)^{n_j} = A(N, \lambda)B(\lambda),\]
where \( N \geq w \),
\[
A(N, \lambda) \sim Binomial(N, 1 - p(0))
\]
and
\[
B(\lambda) \sim Multinomial\left(w, \frac{p(\lambda(j))}{1 - p(0)}\right), j = 1, 2, \ldots.
\]

The joint distribution of \((N, \lambda)\), where \(N\) is the number of species and \(\lambda\) is the parameter for the prior distribution, is
\[
\pi(N, \lambda | \text{Data}) \propto L_M(N, \lambda)\pi(N, \lambda).
\]

If we use the prior \(\pi(N, \lambda) \propto \frac{1}{\lambda} \pi(\lambda)\), we have
\[
\pi(N, \lambda | \text{Data}) \propto \frac{N!}{(N - w)!w!(p(0))^{N-w}} \frac{w!}{n_1!n_2! \cdots} (1 - p(0))^w \prod_{j \geq 1} \left( \frac{p(\lambda(j))}{1 - p(0)} \right)^{n_j} \frac{1}{N} \pi(\lambda)
\]
\[
\propto \frac{(N - 1)!}{(N - w)!(w - 1)!} (p(0))^{N-w} (1 - p(0))^w \frac{w!}{n_1!n_2! \cdots} \prod_{j \geq 1} \left( \frac{p(\lambda(j))}{1 - p(0)} \right)^{n_j} \pi(\lambda)
\]
\[
\propto \left( \begin{array}{c} N - 1 \\ w - 1 \end{array} \right) p_{\lambda}^{N-w}(0)(1 - p(0))^w \left( \begin{array}{c} w \\ n_1, n_2, \ldots \end{array} \right) \prod_{j \geq 1} \left( \frac{p(\lambda(j))}{1 - p(0)} \right)^{n_j} \pi(\lambda).
\]

So, the conditional posterior distribution of \(N\) is proper and is given by
\[
\pi(N | \lambda, \text{Data}) \propto \left( \begin{array}{c} N - 1 \\ w - 1 \end{array} \right) p_{\lambda}^{N-w}(0)(1 - p(0))^w.
\]

This corresponds to the negative binomial distribution for \(N\) with parameters \(w\) and \(1 - p(0)\).

The conditional posterior distribution to \(\lambda\) is:
\[ \pi(\lambda|N, Data) \propto p_N^{N-w}(0) \prod_{j \geq 1} p_{\lambda}^{n_j}(j) \pi(\lambda). \]

We wish to evaluate the posterior distribution of \( N \) and \( \lambda \) based on the Poisson-gamma mixture distribution. We express the prior not as a function of \( \lambda \) but as a function of parameters \( \alpha \) and \( \beta \) as follows:

\[
\theta_i|\alpha, \beta \sim \Gamma \left[ \beta, \frac{1 - \alpha}{\alpha} \right], \quad \lambda = (\alpha, \beta), \beta > 0
\]

where the \( \pi \)-mixture is

\[
p_{\lambda}(j) = \int_0^{\infty} \frac{\theta^j e^{-\theta}}{j!} \pi(\theta|\alpha, \beta) d\theta
\]

\[
= \int_0^{\infty} \frac{\theta^j e^{-\theta}}{j!} \left( \frac{1 - \alpha}{\alpha} \right)^\beta e^{-\left(\frac{1 - \alpha}{\alpha}\right)\theta} \frac{\Gamma(\beta)}{\Gamma(\beta)} d\theta
\]

\[
= \frac{(1 - \alpha)^\beta}{\alpha^\beta \Gamma(\beta) j!} \int_0^{\infty} e^{-\left(\frac{1}{\alpha}\right)\theta} \theta^{\beta+j-1} d\theta
\]

\[
= \frac{(1 - \alpha)^\beta \Gamma(\beta + j)}{\alpha^\beta \Gamma(\beta) j!} \int_0^{\infty} \left( \frac{1}{\alpha} \right)^{\beta+j} \frac{1}{\Gamma(\beta + j)} e^{-\left(\frac{1}{\alpha}\right)\theta} \theta^{\beta+j-1} d\theta
\]

\[
= \frac{(1 - \alpha)^\beta \Gamma(\beta + j)}{\Gamma(\beta)} \frac{1}{j!} \alpha^j = NB[j; \beta, 1 - \alpha],
\]

for \( j = 0, 1, \ldots \). If \( j = 0 \), then we have

\[
p_{\lambda}(0) = (1 - \alpha)^\beta.
\]

We assume the non-informative prior for all parameters \( \pi(N, \alpha, \beta) \propto \frac{1}{N} \), so that the
The joint distribution given the data is

$$\pi(N, \alpha, \beta | \text{Data}) \propto \frac{N!}{(N-w)!w!} ((1-\alpha)^\beta)^{N-w} \frac{w!}{n_1!n_2!} \cdots (1-(1-\alpha)^\beta)^w \prod_{j \geq 1} \left( \frac{(1-\alpha)^\beta \Gamma(\beta+j)}{\Gamma(\beta) j!} \alpha^j \right)^n_j \frac{1}{N}$$

$$\propto \frac{(N-1)!}{(N-w)!((w-1)!)} ((1-\alpha)^\beta)^{N-w} (1-(1-\alpha)^\beta)^w \frac{w!}{n_1!n_2!} \cdots \prod_{j \geq 1} \left( \frac{(1-\alpha)^\beta \Gamma(\beta+j)}{\Gamma(\beta) j!} \alpha^j \right)^n_j$$

$$\propto \left( \begin{array}{c} N-1 \\ w-1 \end{array} \right) ((1-\alpha)^\beta)^{N-w} (1-(1-\alpha)^\beta)^w \left( \begin{array}{c} w \\ n_1, n_2, \ldots \end{array} \right) \prod_{j \geq 1} \left( \frac{(1-\alpha)^\beta \Gamma(\beta+j)}{\Gamma(\beta) j!} \alpha^j \right)^n_j .$$

The conditional posterior distribution of the number of species $N$ given the data, $\alpha$ and $\beta$ is

$$\pi(N | \alpha, \beta, \text{Data}) \propto \left( \begin{array}{c} N-1 \\ w-1 \end{array} \right) ((1-\alpha)^\beta)^{N-w} (1-(1-\alpha)^\beta)^w,$$

which corresponds to the negative binomial distribution for $N$ with parameters $w$ and $1 - (1 - \alpha)^\beta$. This allows for an appropriate interpretation of the conditional distribution $N$ because, this is a random variable that represents the number of Bernoulli trials to obtain $w$ successes. There are at least $w$ successes because these are the observed species in the sample. The probability of observing a species in a sample is $1 - (1 - \alpha)^\beta$. The only difficulty with the Negative Binomial distribution is that it is unbounded.

The conditional posterior for $\alpha$ and $\beta$ are as follows:

$$\pi(\alpha | \beta, N, \text{Data}) \propto ((1-\alpha)^\beta)^{N-w} \prod_{j \geq 1} \left\{ \frac{(1-\alpha)^\beta \Gamma(\beta+j)}{\Gamma(\beta) j!} \alpha^j \right\}^{n_j}$$
\[ \propto (1 - \alpha)^{\beta N} \prod_{j \geq 1} \left\{ \frac{\Gamma(\beta + j)}{\Gamma(\beta)} \alpha^j \right\}^{n_j} \]

\[ \propto (1 - \alpha)^{\beta N} \alpha^n \prod_{j \geq 1} \left\{ \frac{\Gamma(\beta + j)}{\Gamma(\beta)} \right\}^{n_j} \]

\[ \propto \frac{\Gamma(n + 1 + \beta N + 1)}{\Gamma(n + 1)\Gamma(\beta N + 1)} \alpha^n (1 - \alpha)^{\beta N}, \]

which corresponds to the Beta distribution for \( \alpha \) with parameters \( n + 1 \) and \( \beta N + 1 \). This makes making inference for the parameter \( \alpha \) uncomplicated because the conditional posterior of \( \alpha \) is a proper probability distribution, which is the same as the case for \( N \).

The conditional posterior of \( \beta \) is given as

\[ \pi(\beta|\alpha, N, Data) \propto ((1 - \alpha)^\beta)^{N - w} \prod_{j \geq 1} \left\{ \frac{(1 - \alpha)^\beta \Gamma(\beta + j)}{\Gamma(\beta)} \frac{1}{j!} \alpha^j \right\}^{n_j} \]

\[ \propto (1 - \alpha)^{\beta N} \prod_{j \geq 1} \left\{ \frac{\Gamma(\beta + j)}{\Gamma(\beta)} \alpha^j \right\}^{n_j} \]

\[ \propto (1 - \alpha)^{\beta N} \prod_{j \geq 1} \left\{ \frac{(\beta + j - 1)!}{(\beta - 1)!} \right\}^{n_j} \]

\[ \propto (1 - \alpha)^{\beta N} \prod_{j \geq 1} \left[ \prod_{i=1}^{j} (\beta + i - 1) \right]^{n_j}. \]

This conditional posterior is not 'proper' and grids are used to draw samples from this distribution. Rodrigues, Milan and Leite [22] did not use 'grids' to draw \( \beta \) in their procedure.

The Gibbs sample from the joint posterior distribution of \((N, \alpha, \beta)\) can be generated from the conditional distributions above. That is,

1. We first draw \( N \) from the Negative Binomial with parameters \( w \) and \( 1 - (1 - \alpha)^\beta \).
2. Next we draw $\alpha$ from a Beta distribution with parameters $n + 1$ and $\beta N + 1$.

3. Lastly, we draw $\beta$ from its conditional posterior using grids.

From this Gibbs sample, we obtain the point estimate for the number of species, the standard error and 95% credible intervals. The point estimate is the posterior mode of the Gibbs sample, and the bounds of the 95% credible intervals are the 2.5% and 97.5% percentiles of the sample.
Chapter 4

Numerical Examples

4.1 Mount Kenya Experiment

By using the methods from Efron and Thisted and Boneh, Boneh and Caron, as implemented by Ramos and R. Villaflor [21] I will get the following results. First, note that $n_t$ is $n_x$ so that in using the first estimator, which is $\hat{\Delta}(t) = n_1 t - n_2 t^2 + n_3 t^3 - \cdots$, the expected number of insects that would be observed in the rest of the area can be identified as

$$\hat{\Delta}(t) = 8t^1 - 3t^2 + 2t^3 - t^4 + t^5 - 3t^6 + 2t^7 - t^{10} - t^{12} - t^{18}$$

$$+ t^{21} + t^{25} - t^{36} - t^{56} - t^{96} - t^{98} + t^{109} + t^{157} + t^{335}.$$  

Using the second estimator, which is $\hat{\Psi}(t) = \sum_{k=1}^{k_{\text{max}}} N_k e^{-k} - \sum_{k=1}^{k_{\text{max}}} N_k e^{-k(1+t)}$, with $k_{\text{max}} = 335$ and some of the $n_t$’s zero, the estimated number of insects that would be seen in the rest of the area would be

$$\hat{\Psi}(t) = \sum_{k=1}^{k_{\text{max}}} N_k e^{-k} - \sum_{k=1}^{k_{\text{max}}} N_k e^{-k(1+t)}$$

33
\[= 3.482981 - \left( 8e^{-1(1+t)} + 3e^{-2(1+t)} + 2e^{-3(1+t)} + \cdots + e^{-157(1+t)} + e^{-335(1+t)} \right).\]

We now apply the bias reduction algorithm. Table 4.1 shows the summary of the bias-correction iterations. These iterations stops at 9 since the stopping criterion, \(U_{i+1} - U_i < \delta\), where \(\delta = 0.001\), is met. Since we stop at 9, we will get the value of \(U_{11}\) which is 4.040747 as the value of \(U\) in the second estimator, which is \(\hat{\Psi}^*(t) = \hat{\Psi}(t) + Ue^{-\hat{\lambda}^*} + U e^{-\hat{\lambda}^*(1+t)}\). Also note that \(N_1/U = \hat{\lambda}^*\) which is equal to 1.979832. Given these values, the corrected second estimator will be

\[\hat{\Psi}^*(t) = \hat{\Psi}(t) + 4.040747e^{-1.979832} + 4.040747e^{-1.979832(1+t)}.\]

For further illustration, we give some pointwise comparisons between \(\hat{\Delta}(t)\) and \(\hat{\Psi}^*(t)\) for different values of \(t\) as shown in Table 4.2. Notice that as \(t\) becomes larger, the value of \(\hat{\Psi}^*(t)\) approaches 4. Thus, we can say that \(\hat{\Psi}^*(\infty) = 4\). This means that we expect to find 4 new distinct species of insects in addition to the insects that were already observed.
Table 4.1: Bias-Correction Iterations for the Mt. Kenya Data

<table>
<thead>
<tr>
<th></th>
<th>$U_i$</th>
<th>$n_1/U_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.482981</td>
<td>2.296883</td>
</tr>
<tr>
<td>2</td>
<td>3.833271</td>
<td>2.08699</td>
</tr>
<tr>
<td>3</td>
<td>3.958537</td>
<td>2.02049</td>
</tr>
<tr>
<td>4</td>
<td>4.007604</td>
<td>1.996205</td>
</tr>
<tr>
<td>5</td>
<td>4.027413</td>
<td>1.986387</td>
</tr>
<tr>
<td>6</td>
<td>4.035503</td>
<td>1.982405</td>
</tr>
<tr>
<td>7</td>
<td>4.038821</td>
<td>1.980776</td>
</tr>
<tr>
<td>8</td>
<td>4.040185</td>
<td>1.980107</td>
</tr>
<tr>
<td>9</td>
<td>4.040747</td>
<td>1.979832</td>
</tr>
</tbody>
</table>
Table 4.2: Pointwise Comparison for the Estimators of the Mt. Kenya Data, $\hat{\Delta}(t)$ and $\hat{\Psi}^*(t)$

<table>
<thead>
<tr>
<th>$t$</th>
<th>$\hat{\Delta}(t)$</th>
<th>$\hat{\Psi}^*(t)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.771907</td>
<td>0.492694</td>
</tr>
<tr>
<td>0.2</td>
<td>1.494553</td>
<td>0.915673</td>
</tr>
<tr>
<td>0.5</td>
<td>3.436276</td>
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</tr>
<tr>
<td>0.9</td>
<td>4.914095</td>
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<td>1</td>
<td>6.000000</td>
<td>2.820945</td>
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<tr>
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<td>37.49332</td>
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</tr>
<tr>
<td>1.02</td>
<td>790.90709</td>
<td>2.847851</td>
</tr>
<tr>
<td>1.03</td>
<td>20097.9059</td>
<td>2.861061</td>
</tr>
<tr>
<td>2</td>
<td>3.624364</td>
<td></td>
</tr>
</tbody>
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### Table 4.3: Analysis of the Mt. Kenya Data Using Different Upper Bounds

<table>
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<tr>
<th>Upper Bound</th>
<th>Posterior Mode</th>
<th>Standard Error</th>
<th>LCL</th>
<th>UCL</th>
</tr>
</thead>
<tbody>
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<td>3.46702</td>
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<td>49</td>
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<tr>
<td>51</td>
<td>45.27</td>
<td>3.89731</td>
<td>37</td>
<td>50</td>
</tr>
<tr>
<td>52</td>
<td>46.38</td>
<td>3.94861</td>
<td>37</td>
<td>51</td>
</tr>
<tr>
<td>53</td>
<td>47.43</td>
<td>4.04833</td>
<td>38</td>
<td>52</td>
</tr>
<tr>
<td>54</td>
<td>47.68</td>
<td>3.98451</td>
<td>40</td>
<td>53</td>
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<tr>
<td>55.5</td>
<td>49.34</td>
<td>4.19528</td>
<td>41</td>
<td>55</td>
</tr>
<tr>
<td>56</td>
<td>49.34</td>
<td>4.19528</td>
<td>41</td>
<td>55</td>
</tr>
<tr>
<td>57</td>
<td>50.31</td>
<td>4.41232</td>
<td>40</td>
<td>56</td>
</tr>
<tr>
<td>58.5</td>
<td>50.83</td>
<td>5.30305</td>
<td>39</td>
<td>58</td>
</tr>
<tr>
<td>59</td>
<td>50.83</td>
<td>5.30305</td>
<td>39</td>
<td>58</td>
</tr>
<tr>
<td>60</td>
<td>51.64</td>
<td>5.12770</td>
<td>41</td>
<td>59</td>
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</table>
Figure 4.1: Plot: Posterior Mode vs Upper Bound for the Mt. Kenya Data
Figure 4.2: Plot: Standard Error vs Upper Bound for the Mt. Kenya Data
4.2 Mount Mandalagan Experiment

By using the methods from Efron and Thisted and Boneh, Boneh and Caron, I will get the following results. First, note that $N_k$ is $n_x$ so that in using the first estimator, which is $\hat{\Delta}(t) = n_1 t - n_2 t^2 + n_3 t^3 - \cdots$, the expected number of trees that would be observed in the rest of the area can be identified as

$$\hat{\Delta}(t) = 7t^1 - 5t^2 + 3t^3 - 3t^4 - 3t^6 + t^7 + 3t^9 + t^{11} - 6t^{12} + 3t^{13} - t^{14}$$

$$+ t^{15} - t^{16} - t^{18} + 2t^{19} + t^{21} - 2t^{22} + t^{23} - t^{24} - t^{30} - t^{36} + t^{91}.$$

Using the second estimator, which is $\hat{\Psi}(t) = \sum_{k=1}^{k_{\text{max}}} N_k e^{-k} - \sum_{k=1}^{k_{\text{max}}} N_k e^{-k(1+t)}$, with $k_{\text{max}} = 91$ and some of the $N_k$’s zero, the estimated number of trees that would be seen in the rest of the area would be

$$\hat{\Psi}(t) = \sum_{k=1}^{k_{\text{max}}} N_k e^{-k} - \sum_{k=1}^{k_{\text{max}}} N_k e^{-k(1+t)}$$

$$= 3.464921 - \left(7e^{-1(1+t)} + 5e^{-2(1+t)} + 3e^{-3(1+t)} + \cdots + e^{-36(1+t)} + e^{-91(1+t)}\right).$$

We now apply the bias reduction algorithm. Table 4.4 shows the summary of the bias-correction iterations. These iterations stops at 11 since the stopping criterion, $U_{i+1} - U_i < \delta$, where $\delta = 0.001$, is met. Since we stop at 11, we will get the value of $U_{11}$ which is 4.31805 as the value of $U$ in the second estimator, which is $\hat{\Psi}^*(t) = \hat{\Psi}(t) + U e^{-\hat{\lambda}^*} + U e^{-\hat{\lambda}^*(1+t)}$. Also note that $N_1/U = \hat{\lambda}^*$ which is equal to 1.621102. Given these values, the corrected second estimator will be

$$\hat{\Psi}^*(t) = \hat{\Psi}(t) + 4.31805e^{-1.621102} + 4.31805e^{-1.621102(1+t)}.$$

For further illustration, we give some pointwise comparisons between $\hat{\Delta}(t)$ and
\[ \hat{\Psi}^*(t) \] for different values of \( t \) as shown in Table 4.5. Notice that as \( t \) becomes larger, the value of \( \hat{\Psi}^*(t) \) approaches 4. Thus, we can say that \( \hat{\Psi}^*(\infty) = 4 \). This means that we expect to find 4 new distinct species of trees in addition to the trees that were already observed.
Table 4.4: Bias-Correction Iterations for the Mt. Mandalagan

<table>
<thead>
<tr>
<th>$i$</th>
<th>$U_i$</th>
<th>$N_1/U_i$</th>
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</thead>
<tbody>
<tr>
<td>1</td>
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<tr>
<td>2</td>
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<tr>
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<tr>
<td>10</td>
<td>4.317151</td>
<td>1.62144</td>
</tr>
<tr>
<td>11</td>
<td>4.31805</td>
<td>1.621102</td>
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</table>
Table 4.5: Pointwise Comparison for the Estimators of the Mt. Mandalagan Data, $\hat{\Delta}(t)$ and $\hat{\Psi}^*(t)$

<table>
<thead>
<tr>
<th>$t$</th>
<th>$\hat{\Delta}(t)$</th>
<th>$\hat{\Psi}^*(t)$</th>
</tr>
</thead>
<tbody>
<tr>
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<td>0.556445</td>
</tr>
<tr>
<td>0.2</td>
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<tr>
<td>0.9</td>
<td>1.665102</td>
<td>2.949751</td>
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</tr>
<tr>
<td>1.03</td>
<td>8.222532</td>
<td>3.144568</td>
</tr>
<tr>
<td>Upper Bound</td>
<td>Posterior Mode</td>
<td>Standard Error</td>
</tr>
<tr>
<td>-------------</td>
<td>----------------</td>
<td>----------------</td>
</tr>
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<td>55</td>
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<td>16.38034</td>
</tr>
<tr>
<td>135</td>
<td>69.25</td>
<td>16.58427</td>
</tr>
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</table>
Figure 4.3: Plot: Posterior Mode vs Upper Bound for the Mt. Mandalagan Data
4.3 Conclusion

For both data sets, the performance of the Efron and Thisted and Boneh, Boneh, Caron methods for estimating the number of species are similar. Both methods greatly underestimate the number of species in the population, as evidenced by the difference in the expected mode for the Kenya data and the estimates from these two methods.

The Hierarchical Bayesian model from Rodrigues, Milan and Leite, adjusted in some aspects for this project gives more reasonable estimates and credible intervals, which the first two methods do not provide because computation of standard errors
are difficult.

The posterior mode of $N$ increases monotonically as the upper bound increases. However, the standard errors do not behave the same way. The upper bound for the distribution must be known beforehand, provided by an expert or analyst involved in the study. This upper bound cannot be obtained from the sample data. In fact, in most of the credible intervals, the upper limit is almost equal to the set upper bound.
Appendix A

Fortran Code

Fortran was used extensively in this project to perform simulations. Fortran is a general-purpose, procedural, imperative programming language that is especially suited to numeric computation and scientific computing.

The remaining pages in this appendix document the Fortran code used in this project.
real ung(500), wing(500), wwing(500), swing(500),
+ probg(500), probgc(0:500), ppmu(10000, 10), aq(10000)

integer ind(19), nn(19), nc(500), ipermg(500), irank(500)

data ind/1,2,3,4,5,6,7,10,12,18,21,25,46,56,95,98,109,157,335/
data nn/8,3,2,1,1,3,2,1,1,1,1,1,1,1,1,1,1,1,1/

cel = ind(19)
write(6,* ) ncel
do j=1,ncel
   nc(j) = 0
end do
do j=1,19
   nc(ind(j)) = nn(j)
end do
isum1 = 0
isum2 = 0
do j=1,ncel
   isum1 = isum1 + nc(j)
   isum2 = isum2 + j*nc(j)
end do
nw = isum1
ns = isum2
alpha = .5
beta = 2

nran = 45
idum = -5

write(6,* ) 'Load nmc,nthrow,ngap,nbatch,iprint !'
read(5,* ) nmc,nthrow,ngap,lbatch,iprint
write(6,1) nmc,nthrow,ngap,lbatch,iprint
1  format(5i6)
nrem = nmc-nthrow
nval = nrem/ngap
nbatch = nval/lbatch
keep = 0
idum = -5
do 1000 it=1, nmc
    nit = mod(it, iprint)
    if(nit .eq. 0 ) then
        write(6,*) 'it ......',it
    end if
    go to 99999
    Draw big N.
    dum = beta*alog(1-alpha)
    pp = 1-exp(dum)
    icheck = 0
    isum = 0
    do ig=1, nw
        uu = ran1(idum)
        dum = alog(1-uu)/alog(1-pp)
        isum = isum + ceiling(dum)
    end do
    nran = isum
    icheck = icheck + 1
    if(nran .ge. 55) go to 99
    write(6,*) 'icheck',icheck
    Draw alpha.
    dff = ns+1
    call gamdev(idum, dff, dran1)
    dff = beta*nran + 1
    call gamdev(idum, dff, dran2)
    alpha = dran1/(dran1+dran2)
    Draw beta [use grids
    ngrid = 100
    bound1 = 0.
    bound2 = 1.
    din = (bound2-bounded1)/ngrid
    do it1=1,ngrid
        ung(it1) = bound1 + din/2 + (it1-1)*din
    end do
do it1=1,ngrid
rbeta = ung(it1)/(1-ung(it1))
arg1 = rbeta*nran*alog(1-alpha)
sum = 0.
do j=1,nCEL
do i=1,j
  sum = sum + nc(j)*alog(rbeta + i - 1)
end do
end do
arg2 = sum
wing(it1) = arg1 + arg2
wwing(it1) = arg1 + arg2
end do

call sort(ngrid,wwing,ipermg,irankg,swing)
term0 = swing(ngrid)
asum = 0.
do it1=1,ngrid
  asum = asum + exp(wing(it1)-term0)
end do
do it1=1,ngrid
  probg(it1) = exp(wing(it1)-term0)/asum
end do
probgc(0) = 0.
do it1=1,ngrid
  probgc(it1) = probgc(it1-1) + probg(it1)
end do
uu = ran1(idum)
do it1=1,ngrid
  if(uu .gt. probgc(it1-1) .and. uu .le. probgc(it1)) then
    ipick = it1
  end if
end do
write(6,*) 'ipick',ipick
ungg = ung(ipick-1) + (ung(ipick)-ung(ipick-1))*ran1(idum)
beta = ungg/(1-ungg)
if(nit .eq. 0) then
  write(6,*) 'nran alpha beta',nran,alpha,beta
end if
if(it .gt. nthrow) then
  itt = mod(it-nthrow,ngap)
  if( itt .eq. 0 ) then
    keep = keep + 1
    ppmu(keep,1) = nran
    ppmu(keep,2) = alpha
    ppmu(keep,3) = beta
  end if
end if

1000 continue
	npar = 3
c
C Study autocorrelation in Gibbs Sampler.
C
  Do 3310 j=1,npar
c    write(6,3311)
c    write(10,3311)
3311 format(20x,'lag',5x,'correlation',5x,'sterr'/)
  sum= 0.
do 3315 it=1,nval
3315   SUM = SUM + ppmu(it,j)
savg = sum/nval
  sum = 0.
do 3320 it=1,nval
3320   sum = sum + (ppmu(it,j)-savg)**2
  co = sum/nval
do 3325 KKK=1,20
3325   sum = sum + (ppmu(it,j)-savg)*(ppmu(it+kkk,j)-savg)
cors = (sum/nval)/co
  str = sqrt( (nval-kkk)/(nval*(nval+2.) ) )
write(6,3331) j,kkk,cors,str
write(10,3331) j,kkk,cors,str
3331 format(10x,2i10,2f10.4/)
3325 continue
3310 continue

  do it=1,nval
    write(7,'(i5,3f10.5)') it,(ppmu(it,k),k=1,npar)
end do

do k=1,npar
    do it=1,nval
        aq(it) = ppmu(it,k)
    end do
    call monte(lbatch,nbatch,aq,avg, std, bstd, c025, c975)
    write(6, '(i5,5f12.5)') k, avg, std, bstd, c025, c975
    write(8, '(i5,5f12.5)') k, avg, std, bstd, c025, c975
end do

stop
end

c
  include 'allrouma556.f'
c
Bibliography


