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BAYESIAN ESTIMATION OF THE NUMBER OF EQUALLY LIKELY CLASSES IN A POPULATION

by
José Galvão Leite
and
Heleno Bolfarine

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BAYESIAN ESTIMATION OF THE NUMBER OF EQUALLY LIKELY CLASSES IN A POPULATION

José G. Leite e Heleno Bolfarine
Departamento de Estatística - Universidade de São Paulo
Caixa Postal 20570 - Agência Iguatemi
01498 - São Paulo - SP - BRASIL

Summary

The Bayes estimator of the number of classes in a population is considered. Attention is restricted to the case where all classes are equiprobable. An exact expression is obtained for the posterior mode under a noninformative prior. Large sample properties of the posterior mean and higher moments of the posterior distribution are investigated. The strongest results are the convergence of the Bayes estimator and the convergence of the posterior variance to zero.

1. Introduction

A random sample of size n is taken from a multinomial distribution with an unknown but finite number of classes, N. The main object is to estimate N. Practical situations related to the estimation of N are reported in Goodman (1949), Efron and Thisted (1976), Holst (1981) and Esty (1985, 1986). Given N classes, we consider that they are indexed by $1,\dots,N$. Let p_j be the probability that any observation belongs to the j-th class and X_j the number of elements of the j-th class observed in the sample, $j=1,\dots,N$. Clearly $\sum_{j=1}^{N} p_j = 1$. Then, $(X_1,\dots,X_N)$ is multinomially distributed with parameters n and $p_1,\dots,p_N$, that is,

$$P[X_1 = x_1,\dots,X_N = x_N] = \frac{n!}{\prod_{j=1}^{N} x_j!}\prod_{i=1}^{N} p_j^{x_j},$$

where $x_j \in \{0,1,\dots,n\}$, $j=1,\dots,N$ and $\sum_{j=1}^{N} x_j = n$. Let N_r be the number of classes that occur r times in the sample, that is, $N_r = \sum_{j=1}^{N} I_{(X_j=r)}$, $r=1,\dots,n$. Thus, $\sum_{r=1}^{n} rN_r = n$ and $T_n = \sum_{r=1}^{n} N_r$ is the number of distinct classes observed in the sample, with $T_n = 1,2,\dots,min\{n,N\}$. Now, for all $n_j \in \{0,1,\dots,n\}$, $1\le j\le n$, such that $\sum_{r=1}^{n} rn_r = n$, $\sum_{r=1}^{n} n_r = t$ and observing that $X_j = x_j$ if and only if the j-th class occurs exactly x_j times in the sample, it follows that the event

$$(N_1 = n_1,\dots,N_n = n_n) = \bigcup_{x_1,\dots,x_N} (X_1 = x_1,\dots,X_N = x_N), \tag{1}$$

where the union in (1) extends to all x_j, $1\le j\le N$, such that n_1 of the x_j are equal to 1, n_2 of the x_j are equal to 2, ..., n_n of the x_j are equal to n and $N-t$ of the x_j are equal to zero. Thus,

$$P(N_1 = n_1,\dots,N_n = n_n|N) = \sum_{x_1,\dots,x_N} P(X_1 = x_1,\dots,X_N = x_N)$$

$$= \sum_{x_1,\dots,x_N} \frac{n!}{x_1!x_2!\dots x_N!} \prod_{j=1}^{N} p_j^{x_j} \tag{2}$$

$$= \frac{n!}{(1!)^{n_1}(2!)^{n_2}\dots(n!)^{n_n}} \sum \prod_{i\in A_1} p_i \prod_{j\in A_2} p_j^2 \prod_{k\in A_3} p_k^3 \cdots \prod_{l\in A_n} p_l^n,$$

where the summation in (2) is extended over all disjoint subsets $A_1,\dots,A_n$ of $\{1,\dots,N\}$ such that A_1 has n_1 elements, A_2 has n_2, ..., A_n has n_n elements. Suppose now that the classes are equiprobable, that is, $p_1 = p_2 = \dots = p_N = 1/N$. Then, it follows from (2) that

$$P(n_1,\dots,n_n|N) = \frac{N!}{(N-t)!N^n} \frac{n!}{\prod_{r=1}^{n} n_r!(r!)^{n_r}},$$

for all $n_1,\dots,n_n \in \{0,1,\dots,n\}$ such that $\sum_{r=1}^{n} rn_r = n$ and $\sum_{r=1}^{n} n_r = t$, which implies that

$$P(T_n = t|N) = \sum\nolimits^{(*)} P(n_1,\dots,n_n|N)$$

$$= \frac{N!}{(N-t)!N^n} \sum\nolimits^{(*)} \frac{n!}{\prod_{r=1}^{n} n_r!(r!)^{n_r}}, \tag{3}$$

$t = 1,\dots,min\{n,N\}$, where $\sum^{(*)}$ extends over all integer and nonnegative solutions of the equations $\sum_{r=1}^{n} rn_r = n$ and $\sum_{r=1}^{n} n_r = t$. Thus, we may writte

$$P(T_n = t|N) = \frac{N!}{(N-t)!N^n} \mathcal{S}(n,t),$$

$t = 1,\dots,min\{n,N\}$, where $\mathcal{S}(n,t)$ are Stirling numbers of the second kind (see Charalambides and Singh, pg 2540, 2.27).

2. The posterior distribution

For all $t \in \mathcal{N}^* = \{1,2,\dots\}$ such that $1 \le t \le n$ let

$$K(k) = \frac{k!}{(k-t)!k^n}, \quad k \in \mathcal{N}^*, \quad k \ge t, \tag{4}$$

π be a probability function for N and

$$A_{\pi,t} = \{x \in \mathcal{N}^*; x \ge t \quad \text{and} \quad \pi(x) > 0\}.$$

Notice that $K(k)$ is the kernell of the likelihood (3), that is, the smallest value of the likelihood function that depends on the value of N. For all $t \in \mathcal{N}^*$ and $k \in A_{\pi,t}$, the posterior probability function of N is given by

$$\pi(k|T_n = t) = \frac{K(k)\pi(k)}{\sum_{k=t}^{\infty} K(k)\pi(k)}$$

$$= C(n,t)\frac{k!\pi(k)}{(k-t)!k^n}, \tag{5}$$

where

$$C(n,t) = [\sum_{k=t}^{\infty} \frac{k!\pi(k)}{(k-t)!k^n}]^{-1}.$$

Some comments are now in order. First notice that

$$\frac{k!}{(k-t)!k^n} = \frac{k(k-1)\dots(k-t+1)}{k^n} \leq 1, \tag{6}$$

which implies that

$$\sum_{k=t}^{\infty} \frac{k!\pi(k)}{(k-t)!k^n} \leq \sum_{k=t}^{\infty} \pi(k) \leq 1.$$

Thus, $0 < C(n,t) < \infty$ and $\pi(.|T_n = t)$ is well defined. Moreover, it is difficult to define a workable conjugate class of distributions for this problem since, for some sample points, the sum of the likelihood over all possible values of N diverges. If an improper prior is considered for N, that is, π does not define a probability measure in $\mathcal{N}^*$, then $[C(n,t)]^{-1}$ converges if and only if $1 \leq t \leq n-2$, that is, $\pi(.|T_n = t)$ is not defined for $t = n-1$ and $t = n$. For the case where it is well defined, the theorem that follows provides an explicit expression for the mode of the posterior probability function (5).

Theorem 2.1. *Consider the improper uniform prior $\pi(k) = 1$, $k \in \mathcal{N}^*$ and $t \in \mathcal{N}^*$ such that $1 \leq t \leq n-2$, with $n \geq 3$. Hence, the mode, $\hat{k}$, of the posterior probability function (5) is unique and given by*

$$\hat{k} = \begin{cases} 1, & \text{if} \quad t = 1 \\ t + k_t - 1, & \text{if} \quad 1 < t \leq n-2, \end{cases}$$

where

$$k_t = min\{k \in \mathcal{N}^*; \quad (t+k-1)^n < k(t+k)^{n-1}\}. \tag{7}$$

Proof. If $t = 1$, then

$$\pi(k|T_n = t) = \frac{k^{-n+1}}{\sum_{k=1}^{\infty} k^{-n+1}},$$

$k \in \mathcal{N}^*$. Therefore, $\hat{k} = 1$. On the other hand, if $1 < t \leq n-2$, then

$$\pi(k|T_n = t) = \frac{\frac{k!}{(k-t)!k^n}}{\sum_{k=t}^{\infty} \frac{k!}{(k-t)!k^n}},$$

$k \geq t$, which implies that

$$\frac{\pi(k+1|T_n = t)}{\pi(k|T_n = t)} = (1 - \frac{t}{k+1})^{-1}(1 - \frac{1}{k+1})^n,$$

$k \geq t$. Let's now consider the function

$$g(x) = (1 - tx)^{-1}(1 - x)^n,$$

for all $x \in [0, 1/t)$. Notice that the function $g(.)$ is such that, for all $k \geq t$,

$$g(\frac{1}{k+1}) = \frac{\pi(k+1|T_n = t)}{\pi(k|T_n = t)}. \tag{8}$$

Moreover, its first derivative is such that

$$g'(x) = (t - n + (n-1)tx)(1 - tx)^{-2}(1 - x)^{n-1},$$

for all $x \in (0, 1/t)$. Hence,

$$g'(x) < 0 \Longleftrightarrow x < \frac{n-t}{(n-1)t};$$

$$g'(x) = 0 \Longleftrightarrow x = \frac{n-t}{(n-1)t}$$

and

$$g'(x) > 0 \Longleftrightarrow x > \frac{n-t}{(n-1)t},$$

which implies that $g(.)$ is a monotone decreasing function in the interval $[0, (n-t)/(n-1)t]$ and monotone increasing in the interval $[(n-t)/(n-1)t, 1/t)$. Thus, since $g(0) = 1$, $g(.)$ is continuous in the interval $(0, 1/t)$ and

$$\lim_{x \to 1/t^-} g(x) = \infty,$$

it follows that there exists a unique point, x_o, in the open interval $(0, t^{-1})$ such that $g(x_o) = 1$, $g(x) < 1$, for all $x \in (0, x_o)$ and $g(x) > 1$, for all $x \in (x_o, t^{-1})$. We note now that the root x_o is not of the form $x_o = 1/k$, $k \in \mathcal{N}^*$. Indeed, if $x_o = 1/k$ for some $k \in \mathcal{N}^*$, then $k > t$ and

$$g(\frac{1}{k}) = (1 - \frac{t}{k})^{-1}(1 - \frac{1}{k})^n = 1$$

is equivalent to

$$\sum_{j=1}^{n-1} \binom{n}{j} (-1)^{n-j} k^{j-1} + k^{n-2} t = \frac{(-1)^{n+1}}{k}.$$

Note that the left hand side of this equation is an integer. However, the right hand side can not be an integer. Thus, $x_o \neq 1/k$ and we can conclude that there is an integer $k_o \in \mathcal{N}^*$ such that $g(1/(t+k)) > 1$, for all $k < k_o$ $(k \in \mathcal{N}^*)$ and $g(1/(t+k)) < 1$, for all $k \geq k_o$ $(k \in \mathcal{N}^*)$. This implies that

$$k_o = min\{k \in \mathcal{N}^*; g(\frac{1}{k+t}) < 1\}$$

$$= min\{k \in \mathcal{N}^*; (t+k-1)^n < k(t+k)^{n-1}\}$$

$$= k_t.$$

Now, from (9), we note that

$$\pi(t+k_t-1|T_n=t) > \pi(t+k_t-2|T_n=t) > \ldots > \pi(t|T_n=t)$$

and

$$\pi(t+k_t-1|T_n=t) > \pi(t+k_t|T_n=t) > \pi(t+k_t+1|T_n=t) > \ldots.$$

Thus, $\hat{k} = t + k_t - 1$ is the unique mode of the posterior probability function (5). This concludes the proof.

A similar argument can be used to show that the maximum likelihood estimator of k, that is, the value of k that maximizes the likelihood (3), is given by

$$\hat{k}_M = \begin{cases} \infty & \text{if } t = n \\ t + k_t - 1 & \text{if } t < n, \end{cases} \tag{9}$$

where k_t is as given in (7). Notice that $\hat{k}_M$ is defined for all values of t. Moreover, it is very simple to implement computer programs in any language, which can be used to find k_t given by (7).

3. Posterior Moments

In this section, we study the case where the prior π is proper and has finite r-th moment, $r \in \mathcal{N}^*$. Condition (6) then implies, for all $t \in \mathcal{N}^*$ such that $1 \le t \le n$ and $A_{\pi,t} \neq \emptyset$, that the r-th moment of the posterior probability function is finite and given by

$$M_r(n,t) = E[N^r|T_n = t]$$

$$= C(n,t) \sum_{k=t}^{\infty} \frac{k!\pi(k)}{(k-t)!k^{n-r}}$$

$$= \frac{C(n,t)}{C(n-r,t)}.$$

In particular, if the first moment of $\pi(k)$ is finite, it follows for all $t \in \mathcal{N}^*$ such that $1 \le t \le n$ and $A_{\pi,t} \neq \emptyset$ that the Bayes estimator of N with repect to the squared error loss is given by

$$E(n,t) = M_1(n,t) = \frac{C(n,t)}{C(n-1,t)}. \tag{10}$$

Before discussing some properties of the posterior moments, we present an example with a Poisson prior distribution.

Example 3.1. In this example, we consider the case where the prior probability distribution for N is Poisson with parameter λ, namely,

$$\pi(k) = \frac{e^{-\lambda}\lambda^k}{k!},$$

$k = 0, 1, \ldots$. Thus, it follows from (10) that the Bayes estimator of N is given by

$$E(n,t) = \frac{\sum_{k=t}^{\infty} \frac{\lambda^k}{(k-t)!k^{n-1}}}{\sum_{k=t}^{\infty} \frac{\lambda^k}{(k-t)!k^{n}}} = \frac{E[(X+t)^{-n+1}]}{E[(X+t)^{-n}]}, \tag{11}$$

$t = 1, \ldots, n$, where X is a random variable with Poisson distribution with parameter λ. Table 1 presents the values of the Bayes estimator for $\lambda = 20$ and $n = 10$ and $n = 15$ and several values of t. In parenthesis we present the MLE $\hat{k}_M$ which follows from (9) and coincides with the Bayes estimator if $t < n - 1$ and $\pi(k) = 1$, for all k.

Table 1. BE (and MLE) of N for Poisson prior with $\lambda = 20$

t	$n = 10$	$n = 15$
1	1.0450 (1)	1.0006 (1)
3	10.2049 (3)	3.5704 (3)
5	15.2625 (5)	8.9280 (5)
9	21.5481 (42)	17.5215 (12)
10	22.90.85 (∞)	19.1690 (16)
14	-	25.0023 (100)
15	-	26.3430 (∞)

Note that the influence of the prior is stronger when the data is less informative, that is, when t is large.

4. Some properties of the posterior moments

In this section we restrict attention to proper prior distributions with finite r-th moment. For all $n \geq 2$ and $r \in \mathcal{N}^*$, recall that the moments of order r (r fixed), namely, $M_r(n,t)$, of the posterior probability function is a funciton of (n,t), where $t \in \mathcal{N}^*$, $1 \leq t \leq n$ and $A_{\pi,t} \neq \phi$. The next result shows that the r-th posterior moment of N is a nonincreasing function of n, for fixed t.

Proposition 4.1. *For all prior probability function π of N with finite r-th moment ($r \in \mathcal{N}^*$), for all $n \geq 2$ and for all $t \in \mathcal{N}^*$, such that $1 \leq t \leq n$ and $A_{\pi,t} \neq \emptyset$, we have that*

$$M_r(n,t) \geq M_r(n+1,t). \tag{12}$$

Equality holds in (12) if the posterior probability function, in (5) is degenerated.

Proof. For all $t \in \mathcal{N}^*$ such that $1 \leq t \leq n$ and $A_{\pi,t} \neq \emptyset$, consider the function $h(.)$ defined in $\mathcal{N}^*$ by

$$h(k) = \begin{cases} 0 & \text{if } k < t \\ \frac{1}{k} & \text{if } k \geq t \end{cases}.$$

Since the function $h(.)$ when restricted to the set $A_{\pi,t}$ is decreasing, it follows (Lehmann, 1966) that

$$E[N^r h(N)|T_n = t] \leq E[N^r|T_n = t]E[h(N)|T_n = t]. \tag{13}$$

Moreover,

$$E[h(N)|T_n = t] = C(n,t)\sum_{k=t}^{\infty} \frac{k!\pi(k)}{(k-t)!k^{n+1}}$$

$$= \frac{C(n,t)}{C(n+1,t)} \tag{14}$$

and

$$E[N^r h(N)|T_n = t] = C(n,t)\sum_{k=t}^{\infty} \frac{k^r k!\pi(k)}{(k-t)!k^{n+1}}$$

$$= \frac{C(n,t)}{C(n+1,t)}E[N^r|T_{n+1} = t] = \frac{C(n,t)}{C(n+1,t)}M_r(n+1,t). \tag{15}$$

Thus, from (13), (14) and (15), it follows that

$$\frac{C(n,t)}{C(n+1,t)}M_r(n+1,t) \leq \frac{C(n,t)}{C(n+1,t)}M_r(n,t),$$

which completes the proof.

From (12) it follows that, if $r = 1$ then,

$$E(n,t) \geq E(n+1,t),$$

which implies that the Bayes estimator of N is a nonincreasing function of n for fixed t, as would be expected. The next result shows that $M_r(n,t)$ is a nondecreasing function of t, for fixed n.

Proposition 4.2. *Let π be a prior probability function of N with finite $(r+1)$-th moment ($r \in \mathcal{N}^*$). For all $n \geq 2$ and all $t \in \mathcal{N}^*$ such that $1 \leq t \leq n-1$ and $A_{\pi,t} \neq \emptyset$, if $\pi(.|T_n = t)$, then*

$$M_r(n,t) \leq M_r(n,t+1). \tag{16}$$

Equality in (16) holds if $\pi(.|T_n = t)$ is degenerate at any point but t.

Proof. For all $t \in \mathcal{N}^*$ such that $1 \leq t \leq n-1$, $A_{\pi,t} \neq \emptyset$ and $\pi(.|T_n = t)$ not degenerate at the point t, we have

$$E[N^r(N-t)|T_n = t] = C(n,t)\sum_{k=t+1}^{\infty} \frac{k^r k!\pi(k)}{(k-t-1)!k^n} = \frac{C(n,t)}{C(n,t+1)}M_r(n,t+1) \tag{17}$$

and

$$E[N-t|T_n=t]=C(n,t)\sum_{k=t+1}^{\infty}\frac{k!\pi(k)}{(k-t-1)!k^n}=\frac{C(n,t)}{C(n,t+1)}. \tag{18}$$

Thus, (17) and (18) imply that

$$\frac{C(n,t)}{C(n,t+1)}[M_r(n,t+1)-M_r(n,t)]$$

$$=E[N^r(N-t)|T_n=t]-E[N-t|T_n=t]E[N^r|T_n=t]$$

$$=E[N^{r+1}|T_n=t]-E[N|T_n=t]E[N^r|T_n=t]$$

$$=Cov[N,N^r|T_n=t]\geq 0$$

(see Lehmann, 1966), which concludes the proof.

In particular, if $r=1$, then

$$E(n,t)\leq E(n,t+1),$$

is a nondecreasing function of t, for fixed n, which also should be expected.

We discuss now two asymptotic properties related to the sequence of posterior moments. The first states that the sequence $M_r(n,t)$ is convergent and stablishes its limit. The second is related to the convergence of the posterior variance.

Theorem 4.1. *For any prior distribution π of N, for all $r,t\in\mathcal{N}^*$ such that $A_{\pi,t}\neq\emptyset$, the sequence $\{M_r(n,t)\}_{n\geq t+r}$ converges. Moreover,*

$$\lim_{n\to\infty}M_r(n,t)=m^r,$$

where $m=minA_{\pi,t}$.

Proof. If $\pi(.|T_n=t)$ is degenerate for $n=t+r$, then $M_r(n,t)=m^r$, for all $n\geq t+r$ and the result follows. If $\pi(.|T_n=t)$ is not degenerate then, for all $n\geq t+r$ we have that

$$M_r(n,t)=\frac{\sum_{k=m}^{\infty}\frac{k^r k!\pi(k)}{(k-t)!k^n}}{\sum_{k=m}^{\infty}\frac{k!\pi(k)}{(k-t)!k^n}}$$

$$=\frac{m^r+\frac{(m-t)!}{m!\pi(m)}\sum_{k=m+1}^{\infty}\frac{k!\pi(k)}{(k-t)!k^{-r}}(\frac{m}{k})^n}{1+\frac{(m-t)!}{m!\pi(m)}\sum_{k=m+1}^{\infty}\frac{k!\pi(k)}{(k-t)!}(\frac{m}{k})^n}.$$

Notice that, for $n\geq t+r$,

$$\sum_{k=m+1}^{\infty}\frac{k!\pi(k)}{(k-t)!k^{-r}}(\frac{m}{k})^n=m^{t+r}\sum_{k=m+1}^{\infty}\frac{k!\pi(k)}{(k-t)!k^t}(\frac{m}{k})^{n-t-r}$$

$$\leq m^{t+r} \sum_{k=m+1}^{\infty} \pi(k)(\frac{m}{k})^{n-t-r} \leq m^{t+r}(\frac{m}{m+1})^{n-t-r} \sum_{k=m+1}^{\infty} \pi(k)$$

$$< m^{t+r}(\frac{m}{m+1})^{n-t-r} = (m+1)^{t+r}(\frac{m}{m+1})^{n} \rightarrow 0,$$

as $n \rightarrow 0$. Similarly, for $n \geq t+r$,

$$\sum_{k=m+1}^{\infty} \frac{k!\pi(k)}{(k-t)!}(\frac{m}{k})^{n} = m^{t} \sum_{k=m+1}^{\infty} \frac{k!\pi(k)}{(k-t)!k^{t}}(\frac{m}{k})^{n-t}$$

$$\leq m^{t}(\frac{m}{m+1})^{n-t} \sum_{k=m+1}^{\infty} \pi(k) < (m+1)^{t}(\frac{m}{m+1})^{n} \rightarrow 0,$$

as $n \rightarrow \infty$, which proves the result.

The convergence of the Bayes risk to zero is considered next.

Theorem 4.2. *For any prior π of N and for all $t \in \mathcal{N}^*$ such that $A_{\pi,t} \neq \emptyset$, the sequence $\{Var[N|T_n = t]\}_{n \geq t+2}$ converges and*

$$\lim_{n \rightarrow \infty} Var[N|T_n = t] = 0. \tag{19}$$

Proof. From Theorem 4.1 it follows that the sequences $\{M_2(n,t)\}_{n \geq t+2}$ and $\{M_1(n,t)\}_{n \geq t+1}$ are convergent and

$$M_2(n,t) \rightarrow m^2 \qquad \text{and} \qquad M_1(n,t) = E[n,t] \rightarrow m,$$

as $n \rightarrow \infty$, where $m = minA_{\pi,t}$. Thus,

$$Var[N|T_n = t] = M_2(n,t) - (M_1(n,t))^2 \rightarrow m^2 - m^2 = 0,$$

as $n \rightarrow \infty$, as was to be proved.

Since

$$Var[N] = Var\{E[N|n,t]\} + E\{Var[N|n,t]\}, \tag{20}$$

it follows from (19) above that as n increasis (and so thus the sample information) the predictive (marginal) variance of N also increasis. Note that the Bayes estimator would be perfect if $E[N|n,t](= E(n,t))$ is equal to N, so that, from (20), the maximum variance would have been attained.

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