AN ASYMPTOTIC LOWER BOUND FOR
THE ENTROPY OF DISCRETE POPULATIONS
WITH APPLICATION TO THE ESTIMATION OF
ENTROPY FOR UNIFORM POPULATIONS

L. B. Cobb and Bernard Harris

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ABSTRACT

In this paper we obtain an asymptotic lower bound for the entropy of a multinomial population with an unknown and perhaps countably infinite number of classes. This bound is a function of the first \( k + 1 \) occupancy numbers of a random sample, and is a useful estimator when most of the sample information is contained in the low order occupancy numbers.
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1. Introduction and Summary. Assume that a random sample of size
N has been drawn from a multinomial population with an unknown and
perhaps countably infinite number of classes. That is, if $X_j$ is the $j$th
observation, and $M_j$ the $j$th class, then

$$P(X_j = M_j) = p_j, \quad j = 1, 2, \ldots; \quad j = 1, 2, \ldots, N$$

and $\sum_j p_j = 1$. The classes are not assumed to have a natural ordering.

Let $n_i$ be the number of classes which occur exactly $i$ times in the
sample. Then $\sum_i (i - 1) n_i = N$. Therefore, the entropy of the population by

$$H(p_1, p_2, \ldots) = \sum_j p_j \log p_j \tag{1}$$

it is shown that for the cumulative distribution function $F^\Psi(x)$, defined by

$$F^\Psi(x) = \sum_{p_j \leq x} \frac{-Np_j}{N \log (\sum_j Np_j)} \tag{2}$$

we have

$$H(p_1, p_2, \ldots) \approx \frac{1}{N} \Psi^\prime(p_1) \int_{-\infty}^{\infty} \frac{1}{x} \log \frac{x}{2\pi e \Psi^2(p_1)} \Psi^\Psi(x) \, dx \tag{3}$$

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In addition, in Harris [1], it is shown that the moments of $F^*(x)$, $\mu_1, \mu_2, \ldots$, are approximately given by

$$
\mu_r \sim \frac{(r+1)! E(n_{r+1})}{E(n_1)}.
$$

If we then replace the expected values in (4) by the observed values, defining

$$
m_r = \frac{(r+1)! n_{r+1}}{n_1},
$$

estimates of the moments of $F^*(x)$ are obtained. Then, let

$$
\mathcal{F}(a\mathbb{I}b) \{m_1, m_2, \ldots, m_k\}
$$

be the set of cumulative distribution functions with $F(a) = 0, F(b) = 1$, and

$$
\int_{-\infty}^{\infty} x^j dF(x) = m_j, \quad j = 1, 2, \ldots, k.
$$

Since $p_1, p_2, \ldots$ are all assumed to be unknown, $F^*(x)$ is unknown, and an asymptotic lower bound to (3) may be found by minimizing

$$
\int_{-\infty}^{\infty} e^x \log \left( \frac{N}{x} \right) dF(x)
$$

over the set $\mathcal{F}(0, N) \{m_1, m_2, \ldots, m_k\}$. This process uses only the information contained in the first $k+1$ occupancy numbers $n_1, n_2, \ldots, n_{k+1}$, and is particularly useful, when the sample information concerning the parameters $p_1, p_2, \ldots$ is concentrated in the low order occupancy numbers. This occurs, for example, if as $N \to \infty$, $p_j \to 0$, $j = 1, 2, \ldots$, in such a way that $0 \leq Np_j < \lambda$, where $\lambda$ is approximately $k+1$. 

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The minimum is explicitly computed for $k = 2$. The process employed here is compared with the maximum likelihood estimates of entropy for uniform populations with $p_j = \frac{1}{M}$, $j = 1, \ldots, M$ and $M \to \infty$ as $N \to \infty$, so that $N/M \to \lambda > 0$.

2. The computation of the lower bound for entropy. In Harris [1], it was shown that for $r^2 = O(N)$ as $N \to \infty$,

$$E(n_r) \sim \frac{1}{r!} \sum_{j=1}^{\infty} (Np_j)^r e^{-Np_j},$$

where the approximation is valid, in the sense that, either both sides are negligible, or the ratio of the two sides approaches unity.

In particular,

$$E(n_1) \sim \sum_{j=1}^{\infty} Np_j e^{-Np_j};$$

hence

$$\frac{1}{N} E(n_1) \int_{-\infty}^{\infty} e^x \log \left( \frac{N}{x} \right) dF(x)$$

$$\sim \frac{1}{N} \sum_{j=1}^{\infty} e^{-Np_j} \log \left( \frac{1}{p_j} \right) Np_j e^{-Np_j}$$

$$= H(p_1, p_2, \ldots).$$

Let $h(x) = e^x \log \frac{N}{x}$. Then we wish to determine $F_0(x) \in \mathcal{F} \left[ 0, N \right]_{\left( m_1, m_2 \right)}$ such that

$$\min_{F(x) \in \mathcal{F} \left[ 0, N \right]_{\left( m_1, m_2 \right)}} \int_{-\infty}^{\infty} h(x) dF(x) = \int_{-\infty}^{\infty} h(x) dF_0(x).$$
Since \( h(0) \) does not exist, we consider instead \( h_{[\epsilon, N]} \), where \( \epsilon > 0 \), is arbitrary. Then \( h(x) \) is bounded on \([\epsilon, N]\) for every \( \epsilon > 0 \) and it is well-known [1] that \( F_{\epsilon}(x) \) defined by

\[
\min_{F(x) \in \mathcal{F}[\epsilon, N]} \int_{-\infty}^{\infty} h(x) \, dF(x) = \int_{-\infty}^{\infty} h(x) \, dF_{\epsilon}(x),
\]

is obtainable as a discrete cumulative distribution function with at most three jumps, say at \( x_1, x_2, x_3 \), \( \epsilon \leq x_1 < x_2 < x_3 \leq N \). Hence, there exists \( \lambda_1, \lambda_2, \lambda_3 > 0 \), \( \sum_{i=1}^{3} \lambda_i = 1 \), with

\[
\begin{align*}
\lambda_1 x_1 + \lambda_2 x_2 + \lambda_3 x_3 &= m_1 \\
\lambda_1^2 x_1^2 + \lambda_2^2 x_2^2 + \lambda_3^2 x_3^2 &= m_2,
\end{align*}
\]

such that

\[
F_{\epsilon}(x) = \begin{cases} 
0, & x < x_1 \\
\lambda_1, & x_1 \leq x < x_2 \\
\lambda_1 + \lambda_2, & x_2 \leq x < x_3 \\
1, & x \geq x_3
\end{cases}
\]

whenever \( m_2 \geq m_1 \), a condition which we will assume throughout the remainder of this discussion. With no loss in generality, we may assume that \( m_2 > m_1 \), since otherwise \( F_{\epsilon}(x) \) is a cumulative distribution function with exactly one jump, and (8) has a trivial solution.

It can be shown that \( \lambda_i > 0 \), \( i = 1, 2, 3 \), if and only if
(11) \((-1)^{i+j}(-x_i x_j - m_i(x_i + x_j) + m_2) \geq 0, \quad 1 \leq i < j \leq 3.\)

In addition, from Harris [1], there exist real numbers \(\alpha_0, \alpha_1, \alpha_2\) such that \(x_1, x_2,\) and \(x_3\) are roots of

(12) \[g(x) = \sum_{i=0}^{2} \alpha_i x^i - h(x) = 0,\]

and

(13) \[\sum_{i=0}^{2} \alpha_i x^i - h(x) \leq 0, \quad x \leq x \leq N.\]

From (11) and (12), we also have that for \(s < x_1 < N, 1 = 1, 2, 3;\)

(14) \[g'(x_1) = \alpha_1 + 2\alpha_2 x_1 - h'(x_1) = 0.\]

To solve (9), (12), (13) and (14), observe that there exist numbers \(\delta_1, \delta_2, \delta_3, 0 < \delta_1 < \delta_2 < \delta_3 < N,\) such that

\[
h''(x) \begin{cases} < 0, & 0 < x < \delta_1 \\ > 0, & \delta_1 < x < \delta_3 \\ < 0, & \delta_3 < x < N \end{cases},
\]

and

\[
h'''(x) \begin{cases} > 0, & 0 < x < \delta_2 \\ < 0, & \delta_2 < x < N \end{cases},
\]

with

\[
\delta_1 \to 0, \quad N \to \infty
\]
\[
\delta_2 = (N-2) + O(\frac{1}{N}), \quad N \to \infty
\]
\[
\delta_3 = (N-1) + O(\frac{1}{N}), \quad N \to \infty
\]
and \( h''(x) \) is strictly decreasing on \((0, \delta_1)\) and \((\delta_2, N)\). We now establish the following

**Lemma.** If \( \epsilon < x_1 < x_2 < N \) \((0 < \epsilon < \delta_1)\), the following conditions cannot be satisfied simultaneously

\[
\begin{align*}
\text{(15)} & : \sum_{i=0}^{L} a_i x_i^1 \leq h(x), \\ 
\text{(16)} & : \sum_{i=0}^{L} a_i x_j^1 = h(x_j), \\ & \quad j = 1, 2.
\end{align*}
\]

**Proof.** Assume (15) and (16) hold. Let \( p(x) = \Sigma_{i=0}^{L} a_i x_i^1 \). Then

\[
\text{(17)} \quad h'(x) = p'(x_j), \quad j = 1, 2.
\]

Let \( I_1 = (\epsilon, \delta_1) \), \( I_2 = (\delta_1, \delta_2) \), \( I_3 = (\delta_2, N) \). Assume \( a_2 > 0 \). Then if \( x_2 \in I_3 \), since \( p(x) \) is strictly convex and \( h(x) \) is strictly concave in \( I_3 \), by (16) and (17), we have \( p(x_0) > h(x_0) \) for some \( x_0 \in I_3 \), contradicting (15). If \( x_2 \in I_2 \), then \( p'(x_2) > 0 \), hence \( p(N) > p(x_2) > 0 = h(N) \), contradicting (15).

If \( x_2 \in I_1 \), then \( \epsilon < x_1 < x_2 < \delta_1 \), and by (16) and Rolle’s Theorem, there exist \( \xi_1, \xi_2, \) \( x_1 < \xi_1 < \xi_2 < x_2 \) such that \( g''(\xi_j) = 0, \ j = 1, 2 \). This, however, implies that \( h''(\xi_j) = 2a_2, \ j = 1, 2 \), contradicting the monotonicity of \( h''(x) \).

If \( a_2 < 0 \), the argument is similar. The case \( a_2 = 0 \) is trivial.

We now obtain \( F_0(x) \).

**Theorem 1.** There exists a unique cumulative distribution function

\[
F_0(x) = \Phi[0, N]_{(m_1, m_2)} \quad \text{such that}
\]

\[
\int_{-\infty}^{\infty} h(x) dF_0(x) = \min_{F(x) \in \Phi[0, N]} \int_{-\infty}^{\infty} h(x) dF(x)
\]
given by

\[
F_0(x) = \begin{cases} 
0 & , 
\frac{Nm_1 - m_2}{N-m_1} 
\leq x \leq \frac{Nm_1 - m_2}{N-m_1} 
\frac{(N-m_1)^2}{(N-m_1)^2 + (m_2 - m_1)^2} \quad , 
x < \frac{Nm_1 - m_2}{N-m_1} 
\frac{Nm_1 - m_2}{N-m_1} 
\leq x < N 
1 & , 
x \geq N
\end{cases}
\]

Proof. By the above lemma, we have \( x_1 = \epsilon, \epsilon < x_2 < N, x_3 = N \).

From (11), we have

\[
\frac{Nm_1 - m_2}{N-m_1} \leq x_2 \leq \frac{m_2 - m_1}{m_1 - \epsilon}.
\]

Thus, by (9), we have

\[
\lambda_1(x_2, \epsilon) = \frac{Nx_2 - m_1(N + x_2) + m_2}{(x_2 - \epsilon)(N - \epsilon)},
\]

\[
\lambda_2(x_2, \epsilon) = \frac{-\epsilon N - m_1(N + \epsilon) + m_2}{(x_2 - \epsilon)(N - x_2)},
\]

and

\[
\lim_{\epsilon \to 0} \lambda_1(x_2, \epsilon) = \frac{Nx_2 - m_1(N + x_2) + m_2}{x_2 N},
\]

\[
\lim_{\epsilon \to 0} \lambda_2(x_2, \epsilon) = \frac{Nm_1 - m_2}{x_2(N - x_2)}.
\]

This gives a parametric family of cumulative distribution functions \( F_{0, x_2}(x) \).

Since \( \lim_{x \to 0^+} h(x) = \infty \), we must have \( \lambda_1(x_2, \epsilon) = O(\frac{1}{h(\epsilon)}), \epsilon \to 0 \), since otherwise \( F_\epsilon(x) \) would not satisfy (8). Hence \( \lim_{\epsilon \to 0} \lambda_1(x_2, \epsilon) = 0 \) and \( \lim_{\epsilon \to 0} \lambda_2(x_2, \epsilon) = \frac{Nm_1 - m_2}{x_2(N - x_2)} \).
\[ x_2 \rightarrow \frac{N m_1 - m_2}{N - m_1} \text{ as } \varepsilon \to 0. \text{ Since } \lambda_1(x_2, \varepsilon) h(\varepsilon) > 0 \text{ for every } \varepsilon > 0, \text{ it follows that } \lambda_1(x_2, \varepsilon) = o\left(\frac{1}{h(\varepsilon)}\right) \text{ as } \varepsilon \to 0, \text{ establishing the theorem.} \]

Finally we have:

**Theorem 2.** The required lower bound for the entropy is

\[
\frac{n_1}{N} \int_{-\infty}^{\infty} h(x) \, dF_0(x) = \frac{n_1}{N} \frac{(N-m_1)^2}{(N-m_1)^2 + (m_2^2 - m_1^2)} e^{\frac{\sqrt{m_1 - m_2}}{N - m_1}} e^{\frac{N(N-m_1)}{\log(N - m_1)}}.
\]

**Remark.** Krein [2] has studied minimization problems similar to (8). However, Krein's methods require that \(1, x, x^2, h(x)\) form a Tschebycheffian system of functions on \([\varepsilon, N]\). A necessary condition for the above (see Pólya and Szegö [3]) is that the Wronskians

\[
W(x) = \begin{vmatrix}
1 & x & x^2 & h(x) \\
0 & 1 & 2x & h'(x) \\
0 & 0 & 2 & h''(x) \\
0 & 0 & 0 & h'''(x)
\end{vmatrix}, \quad \varepsilon \leq x \leq N,
\]

be non-negative (non-positive) on \([\varepsilon, N]\). This condition is clearly not satisfied in this case and Krein's methods are therefore inapplicable.

3. **The Estimation of the Entropy of Uniform Populations.** Let

\[
p_j = \begin{cases}
\frac{1}{M} & \text{if } j = 1, 2, \ldots, M \\
0 & \text{otherwise}
\end{cases}
\]
Then,

\[
F^*(x) = \begin{cases} 
0 & x < N/M \\
1 & x \geq N/M 
\end{cases}
\]

Note:

\[N \to \infty, \quad M \to \infty \quad \text{so that} \quad N/M \to \gamma > 0.\]

Then,

\[
L(n_i) = \frac{M}{r} \lambda^r e^{-\lambda} \quad r = 1, 2, \ldots
\]

and

\[
\mu_i - \lambda^r = \gamma^r \quad r = 1, 2, \ldots
\]

In the case

\[
\frac{1}{N} \sum_{r=1}^{\infty} \ln(n_r) \int_{x_r}^{\infty} \ln(x) dF^*(x) = e^{-\lambda} \ln(\lambda) - \log M
\]

as required.

In addition, the class \( \pi \left( \frac{N}{r}, \frac{M}{r} \right) \) contains only \( F^*(x) \), so that the

solution of (6) provides an estimation of \( H(p_1, p_2, \ldots) \) rather than a lower bound.

In the replacement of \( \mu_i \), \( \mu_j \) by the sample quantities \( m_i, m_j \), it may

happen that \( m_j < m_i \). This, of course, suggests that \( F^*(x) \) is degenerate,

and in such cases, we take \( m_i = m_j \).

By way of contrast, the maximum likelihood estimate \( \hat{H}(p_1, p_2, \ldots) \) for \( H(p_1, p_2, \ldots) \)

the limiting process employed in the case when
\[ E(\hat{H}) = \sum_{i=1}^{N} E(n_i) \frac{1}{N} \log \left( \frac{1}{N} \right) \]

and for \( M = 1000, N = 100 \), we have \( E(n_1) = 90.48, E(n_2) = 4.52, E(n_3) = 0.15 \)

obtaining

\[ E(\hat{H}) = 4.271 \]

and \( \log M = 6.908 \).

**Example.** Three random samples were chosen with \( N = 1000, M = 1000 \).

The data are summarized below.

<table>
<thead>
<tr>
<th>Sample #1</th>
<th>Sample #2</th>
<th>Sample #3</th>
</tr>
</thead>
<tbody>
<tr>
<td>( n_1 )</td>
<td>373</td>
<td>341</td>
</tr>
<tr>
<td>( n_2 )</td>
<td>199</td>
<td>179</td>
</tr>
<tr>
<td>( n_3 )</td>
<td>62</td>
<td>70</td>
</tr>
<tr>
<td>( n_4 )</td>
<td>8</td>
<td>17</td>
</tr>
<tr>
<td>( n_5 )</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>( n_6 )</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>( n_7 )</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>( m_1 )</td>
<td>1.067</td>
<td>1.050</td>
</tr>
<tr>
<td>( m_2 )</td>
<td>0.997</td>
<td>1.232</td>
</tr>
<tr>
<td>( \frac{n_1}{N} \int h(x) , dF_0(x) )</td>
<td>( \cdots )</td>
<td>6.683</td>
</tr>
<tr>
<td>( H(p_1, \ldots, p_M) )</td>
<td>6.908</td>
<td>6.908</td>
</tr>
<tr>
<td>( \hat{A} )</td>
<td>6.364</td>
<td>6.294</td>
</tr>
</tbody>
</table>

In sample #1, \( m_2 < m_1 \), then supposing \( F^*(x) \) to be degenerate with a jump of 1 at \( m_1 \), we get, using \( m_2 = m_1, \frac{n_1}{N} \int h(x) \, dF_0(x) = 7.419 \).
REFERENCES


