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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 \( X_i \) is the \( i \)th
observation, and \( M_j \) the \( j \)th class, then

\[
P(X_i = M_j | \mathbf{p}) = p_j \quad i = 1, 2, \ldots; \quad j = 1, 2, \ldots, N
\]

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

Let \( n_j \) be the number of classes which occur exactly \( k \) times in the
sample. Then \( \sum_j n_j = N \).

Defining the entropy of the population by

\[
H(p_1, p_2, \ldots) = \sum p_i \log p_i
\]

it is shown, that for the cumulative distribution function \( F^0(x) \), defined by

\[
F^0(x) = \sum_{n_p \leq x} \frac{Np_i}{N} \left( \sum_{n_p \leq x} \frac{Np_i}{N} \right)
\]

we have

\[
H(p_1, p_2, \ldots) \geq \frac{1}{N} \log \left( \int_{-\infty}^{\infty} \frac{Np_i}{N} \left( \sum_{n_p \leq x} \frac{Np_i}{N} \right) \right)
\]

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Wisconsin, and a grant from the National Science Foundation.
In addition, in Harris [1], it is shown that the moments of \( F^*(x) \), \( \mu_1, \mu_2, \ldots \), are approximately given by

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

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

\[
\mathcal{F}_{[a, b]}(m_1, m_2, \ldots, m_k)
\]

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 \( k + 1 \).
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 $p_j = \frac{1}{M}, \ j = 1, 2, \ldots, M$ 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 $r^2 = 0(N)$ as $N \to \infty$,

\begin{equation}
E(n_i) = \frac{1}{r!} \sum_{j=1}^{\infty} (Np_j)^r e^{-Np_j},
\end{equation}

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,

\begin{equation}
E(n_i) = \sum_{j=1}^{\infty} Np_j e^{-Np_j};
\end{equation}

hence

\begin{align*}
\frac{1}{N} E(n_i) & \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).
\end{align*}

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

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

\[
\min_{\substack{F(x) \in \tau_{[\varepsilon, N]} \cap (m_1, m_2) \cap [m_1, m_2]}} \int_{-\infty}^{\infty} h(x) dF(x) = \int_{-\infty}^{\infty} h(x) dF_\varepsilon(x),
\]

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

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

such that

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

whenever \( m_2 > m_1^2 \), a condition which we will assume throughout the remainder of this discussion. With no loss in generality, we may assume that \( m_2 > m_1^2 \), since otherwise \( F_\varepsilon(x) \) is a cumulative distribution function with exactly one jump, and (8) has a trivial solution.

It can be shown that \( \lambda_1 > 0, \ i = 1, 2, 3 \) if and only if

\[
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\]
\[(11) \quad (-1)^{i+j-1}(x^1_x - m_1(x^1_x + x^2) + m^2) \geq 0, \quad 1 \leq i < j \leq 3.\]

In addition, from Harris \cite{11}, there exist real numbers \(a_0, a_1, a_2\) such that \(x_1, x_2,\) and \(x_3\) are roots of

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

and

\[(13) \quad \sum_{i=0}^{2} a_i x^i - h(x) \leq 0, \quad 1 \leq x \leq N.\]

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

\[(14) \quad g'(x_1) = a_1 + 2a_2 x_1 - h'(x_1) = 0.\]

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

\[
\begin{cases}
< 0, & 0 < x < \delta_1, \\
> 0, & \delta_1 < x < \delta_3, \\
< 0, & \delta_3 < x \leq N.
\end{cases}
\]

and

\[
\begin{cases}
> 0, & 0 < x < \delta_2, \\
< 0, & \delta_2 < x \leq N.
\end{cases}
\]

with

\[
\delta_1 \to 0, \quad N \to \infty
\]

\[
\delta_2 = (N-2) + O\left(\frac{1}{N}\right), \quad N \to \infty
\]

\[
\delta_3 = (N-1) + O\left(\frac{1}{N}\right), \quad N \to \infty
\]
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:

\[
\begin{align*}
(15) & \quad \sum_{i=0}^{2} a_i x_i^4 \leq h(x), \quad \epsilon \leq x \leq N \\
(16) & \quad \sum_{i=0}^{2} a_i x_j^4 = h(x_j), \quad j = 1, 2.
\end{align*}
\]

**Proof.** Assume (15) and (16) hold. Let \( p(x) = \sum_{i=0}^{2} a_i x_i^4 \). Then

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

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

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

\[
\int_{-\infty}^{\infty} h(x) \, dF_0(x) = \min_{F(x) \in \mathcal{F} \left[ 0, N \right]_{\left( m_1, m_2 \right)}} \int_{-\infty}^{\infty} h(x) \, dF(x)
\]
given by

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

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

From (11), we have

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

Thus, by (9), we have

\[
\begin{align*}
\lambda_1(x^2, \epsilon) &= \frac{N x_2 - m_1 (N + x_2) + m_2}{(x_2 - \epsilon)(N - x_2)} \\
\lambda_2(x^2, \epsilon) &= \frac{- (\epsilon N - m_1 (N + \epsilon) + m_2)}{(x_2 - \epsilon)(N - x_2)}
\end{align*}
\]

and

\[
\begin{align*}
\lim_{\epsilon \to 0} \lambda_1(x^2, \epsilon) &= \frac{N x_2 - m_1 (N + x_2) + m_2}{x_2 N} \\
\lim_{\epsilon \to 0} \lambda_2(x^2, \epsilon) &= \frac{N m_1 - m_2}{x_2 (N - x_2)}
\end{align*}
\]

This gives a parametric family of cumulative distribution functions \( F_{\theta, x^2}(x) \).

Since \( \lim_{x \to 0^+} h(x) = \infty \), we must have \( \lambda_1(x^2, \epsilon) = O\left(\frac{1}{h(\epsilon)}\right) \), \( \epsilon \to 0 \), since otherwise \( F_{\theta}(x) \) would not satisfy (8). Hence \( \lim_{\epsilon \to 0} \lambda_1(x^2, \epsilon) = 0 \) and \( \lim_{\epsilon \to 0} \lambda_2(x^2, \epsilon) = \frac{N m_1 - m_2}{x_2 (N - x_2)} \).

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\[ x_2 \sim \frac{Nm_1 - m_2}{N - m_1} \text{ as } \epsilon \to 0. \] Since \( \lambda_1(x_2, \epsilon) h(\epsilon) \geq 0 \) for every \( \epsilon > 0 \), it follows that \( \lambda_1(x_2, \epsilon) = o\left(\frac{1}{h(\epsilon)}\right) \) as \( \epsilon \to 0 \), establishing the theorem.

Finally we have:

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

\[
\frac{n_1}{N} \int_{-\infty}^{\infty} h(x) \, dF_0(x) = \frac{n_1}{N} \frac{(N-m_1)^2}{(N-m_1)^2 + (m_2 - m_1)^2} e^{\frac{Nm_1 - m_2}{N - m_1}} \log \frac{N(N-m_1)}{Nm_1 - m_2}.
\]

**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 \([\epsilon, N]\). A necessary condition for the above (see Pólya and Szegő [3]) is that the Wronskians

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

be non-negative (non-positive) on \([\epsilon, N]\). 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

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

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

Note

\[ N \rightarrow \infty, \quad M \rightarrow \infty \quad \text{so that} \quad N/M + \lambda > 0. \]

Thus,

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

and

\[ \mu_i = \lambda^v \quad i = 1, 2, \ldots \]

In the case

\[ \frac{1}{N} \log L(n_i) \int_{-\infty}^{\infty} \log(x) dF^v(x) = e^{\lambda} \log(n) - \log M \]

as required.

In addition, the class \( \pi \bigg| \left( \mu_1, \mu_2 \right) \) contains only \( F^v(x) \), so that the solution of (5) provides an estimation of \( H(p_1, p_2, \ldots) \) rather than a lower bound.

In the replacement of \( p_1, p_2 \) by the sample quantities \( m_1, m_2 \), it may happen that \( m_2 < m_1^v \). This, of course, suggests that \( F^v(x) \) is degenerate, and in such cases, we take \( m_2 = m_1^v \).

By way of contrast, the maximum likelihood estimate \( \hat{H} \) is probably not the limiting process employed in the case.
\[ E(\hat{H}) = \sum_{i=1}^{N} E(n_i) \frac{1}{N} \log \left( \frac{1}{N} \right) \]

and for \( M = 1000, N = 100 \), we have \( E(n_1) = 90.48, E(n_2) = 4.52, E(n_3) = .15 \)

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>.997</td>
<td>1.232</td>
</tr>
<tr>
<td>( \frac{n_1}{N} \int h(x) , dF_0(x) )</td>
<td>......</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

\[ m_2 = m_1, \quad \frac{n_1}{N} \int h(x) \, dF_0(x) = 7.419. \]
REFERENCES


