Entropy Estimates from Insufficient Samplings

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We present a detailed derivation of some estimators of Shannon entropy for discrete distributions. They hold for finite samples of $N$ points distributed into $M$ “boxes”, with $N$ and $M \to \infty$, but $N/M < \infty$. In the high sampling regime ($\gg 1$ points in each box) they have exponentially small biases. In the low sampling regime the errors increase but are still much smaller than for most other estimators. One advantage is that our main estimators are given analytically, with explicitly known analytical formulas for the biases.

It is well known that estimating (Shannon) entropies from finite samples is not trivial. If one naively replaces the probability $p_i$ to be in “box” $i$ by the observed frequency, $p_i \approx n_i/N$, statistical fluctuations tend to make the distribution look less uniform, which leads to an underestimation of the entropy. There have been numerous proposals on how to estimate the bias, but some make quite strong assumptions [4, 7], others use Bayesian methods [6, 11, 12]. As pointed out in [4, 13], one can devise estimators with arbitrarily small bias (for sufficiently large $N$ and fixed $p_i$), but these will then have very large statistical errors (if sufficiently many of the $n_i$ are small but $\neq 0$). In the present paper we want to revisit a method used in [4]. There a very simple correction term was derived which seems to be a very good compromise between bias, statistical errors, and ease of use. Unfortunately, the treatment in [4] was not quite systematic, and in particular the corrections going beyond the proposed term were wrong. It is the purpose of the present letter to provide a more systematic presentation of the method used in [4], to correct some of the errors made there, and to propose an estimator which is again very easy to use and which should be better than that proposed in [4].

We consider $M \gg 1$ “boxes” (states, possible experimental outcomes, ...) and $N \gg 1$ points or particles distributed randomly and independently into the boxes. We assume that each box has weight $p_i$ ($i = 1, \ldots, M$) with $\sum_i p_i = 1$. Each box $i$ will contain a random number $n_i$ of points, with $E[n_i] = p_i N$. Their distribution is binomial,

$$P(n_i; p_i, N) = \binom{N}{n_i} p_i^{n_i} (1 - p_i)^{N-n_i}. \quad (1)$$

Since entropy $H$ is a sum over terms each of which depends only on one index $i$, we only need these marginal distributions instead of the more complicated and non-factorizing joint distribution. Some of the $p_i$ can be zero, but in the following we shall assume that none of them is large, i.e. $p_i \ll 1$ for all $i$. In that limit the numbers $n_i$ are Poisson distributed,

$$P(n_i; z_i) = \frac{z_i^{n_i}}{n_i!} e^{-z_i}. \quad (2)$$

with $z_i = E[n_i] = p_i N$. The error in going from Eq. (1) to (2) is $O(1/N)$. Thus all derivations given below hold strictly only in the limit $N \to \infty$, $M \to \infty$, $n_i/N \to 0 \forall i$, but the general case is not much more difficult, see footnote [4].

Our aim is to estimate the entropy,

$$H = -\sum_{i=1}^{M} p_i \ln p_i = \ln N - \frac{1}{N} \sum_{i=1}^{M} z_i \ln z_i, \quad (3)$$

from an observation of the numbers $\{n_i\}$ (in the following, all entropies are measured in “natural units”, not in bits). The estimator $\hat{H}(n_1, \ldots, n_M)$ will of course have both statistical errors and a bias, i.e. if we repeat this experiment, the average of $\hat{H}$ will in general not be equal to $H$,

$$\Delta H \equiv E[\hat{H}] - H \neq 0. \quad (4)$$

In the limit $N \to \infty, M \to \infty$, the statistical error will go to zero (because essentially one averages over many boxes), but the bias will remain finite unless also $n_i \to \infty \forall i$ in this limit, which we will not assume in the following. Indeed it is well known that the naive estimator, obtained by assuming $z_i = n_i$ without fluctuations,

$$\hat{H}_{\text{naive}} = \ln N - \frac{1}{N} \sum_{i=1}^{M} n_i \ln n_i, \quad (5)$$

is negatively biased, $\Delta H_{\text{naive}} < 0$.

In the limit of large $N$ and $M$ each contribution $z_i \ln z_i$ to the entropy will be statistically independent, and can thus also be estimated independently by some estimator which is only a function of $n_i$ [4],

$$z_i \ln z_i \approx z_i \ln z_i = n_i \phi(n_i) \quad (6)$$

such that its expectation value is

$$E[z_i \ln z_i] = \sum_{n_i=1}^{\infty} n_i \phi(n_i) P(n_i; z_i). \quad (7)$$

Notice that the sum here runs only over strictly positive values of $n_i$. Effectively this means that we have assumed that observing an outcome $n_i = 0$ does not give any
information: If \( n_i = 0 \), we do not know whether this is because of statistical fluctuations or because \( p_i = 0 \) for that particular \( i \).

The resulting entropy estimator is then

\[
\hat{H}_\phi = \ln N - \frac{M}{N} n\phi(n)
\]

with the overbar indicating an average over all boxes,

\[
n\phi(n) = \frac{1}{M} \sum_{i=1}^{M} n_i \phi(n_i).
\]

Its bias is

\[
\Delta H_\phi = \frac{M}{N} (\bar{z} \ln z - E[n\phi(n)]).
\]

It will turn out that some of the derivations given below simplify if we consider instead of the Shannon case the more general Renyi entropies,

\[
H(q) = \frac{1}{1-q} \ln \left( \sum_{i=1}^{M} p_i^q \right)
= \frac{1}{1-q} \ln \left( \sum_{i=1}^{M} z_i^q - q \ln N \right).
\]

The Shannon case is recovered by taking the limit \( q \to 1 \),

\[
H = \lim_{q \to 1} H(q).
\]

Eqs. (8) to (10) are then replaced by \( z_i^q = n_i \phi(n_i, q) \) with \( \phi(n) = d\phi(n, q)/dq \big|_{q=1}, \)

\[
E[z_i^q] = \sum_{n_i} n_i \phi(n_i, q) \tilde{P}(n_i; z_i),
\]


\[
\Delta \exp((1-q)H(q))_\phi = \frac{M}{N} (\bar{z}^q - E[n\phi(n, q)]).
\]

For integer \( q \geq 2 \), the bias-free estimator is given by (in the following we shall suppress the index \( i \))

\[
\hat{z}^q = \frac{n!}{(n-q)!},
\]

since the factorial moments satisfy

\[
\sum_{n=q}^{\infty} \frac{n!}{(n-q)!} P(n; z) = z^q.
\]

This suggests that it might be a good strategy to look first at the generalization of the l.h.s. for arbitrary \( q \), and then analyze more closely the difference with \( z^q \). In addition, we will see that we should start with negative real \( q \), and go to positive \( q \) only later by analytic continuation.

We thus define

\[
A(-q, z) = \sum_{n=1}^{\infty} \frac{\Gamma(n+1)}{\Gamma(n+1+q)} z^n e^{-z}
= E[\frac{\Gamma(n+1)}{\Gamma(n+1+q)}].
\]

We write \( \Gamma(n+1)/\Gamma(n+1+q) = B(n+1, q)/\Gamma(q) \) and use the integral representation for the beta function (Ref. [15], paragraph 6.2.1)

\[
B(n+1, q) = \int_0^1 dt \ (1-t)^n t^{q-1}.
\]

Since both this integral and the sum over \( n \) in the definition of \( A(-q, z) \) are absolutely convergent, we can interchange them. The sum can then be done exactly, giving

\[
A(-q, z) = \frac{1}{\Gamma(q)} \int_0^1 dt \ t^{q-1} (1-e^{-tz} - e^{-z})
= \frac{z^{-q}}{\Gamma(q)} \int_0^z dx \ x^q e^{-x} - \frac{e^{-z}}{\Gamma(1+q)}.
\]

The last term arises since the sum over \( n \) extends only from 1 to \( \infty \). Writing now \( \int_0^1 = \int_0^\infty - \int_0^1 \) we can express the first term as a Gamma function, and the second as an incomplete Gamma function (Ref. [15], paragraph 6.5.3),

\[
A(-q, z) = z^{-q} \frac{\Gamma(q, z)}{\Gamma(1+q)} - \frac{e^{-z}}{\Gamma(1+q)}.
\]

Here we can finally continue analytically to positive \( q \). Furthermore we use the recursion relation (Ref. [15], paragraph 6.5.22)

\[
\Gamma(a, z) = \frac{1}{a} \Gamma(1+a, z) - \frac{z^{a-1} e^{-z}}{a}
\]

to arrive finally at

\[
E[n\psi(n)] = z \ln z + z E_1(z).
\]

For the Shannon case we take the derivative with respect to \( q = 1 \) and obtain

\[
\Gamma(a, z) = \frac{1}{a} \Gamma(1+a, z) - \frac{z^{a-1} e^{-z}}{a}
\]

\[
E_1(z) = \Gamma(0, x) = \int_1^\infty \frac{e^{-x}}{t} dt
\]

is an exponential integral (Ref. [15], paragraph 5.1.4). Eq. (21) is our first important result. For large values of \( z \), \( z E_1(z) \approx c^{-z} \). Thus, if \( z = E[n] \) is large, it is an exponentially good approximation to simply neglect the last term in Eq. (21).

We call the resulting entropy estimator \( \hat{H}_\psi \).

\[
\hat{H}_\psi = \ln N - \frac{1}{N} \sum_{i=1}^{M} n_i \psi(n_i).
\]

Moreover, for \( z \to 0 \) we have also \( z E_1(z) \to 0 \), and in between 0 and \( \infty \) the function is positive with a single maximum at \( z = 0.434... \) where \( z E_1(z) = 0.2815... \). If
we simply neglect the last term, we make thus a negative bias, but at most by
\[ 0 < -\Delta H_\psi = zE_1(z)M/N < 0.2815 \ldots \times M/N. \] (24)

If we approximate further \( \psi(x) \approx \ln x \), we obtain the naive estimator. The better approximation \( \psi(x) \approx \ln x - 1/2x \) gives Miller’s correction \[ 13 \]. It can be shown that
\[ E[n \ln n] > E[n \ln n - 1/2] > E[n\psi(n)] > z \ln z \] (25)
for all positive \( z \). Thus both the naive estimate and Miller’s correction are worse than \( \hat{H}_\psi \). The difference is especially big for large \( z \), where the error of the naive estimate goes to \( M/2N \), the error after applying Miller’s correction is \( \sim M/2N \), while the error of \( \hat{H}_\psi \) is \( \sim \exp(-z)M/N \).

But we can do even better. First we notice that
\[ -\sum_{n=1}^{\infty} \frac{(-1)^n z^n}{n(n+1)} e^{-z} = e^{-z} - \frac{e^{-z}}{z} + \frac{e^{-2z}}{z} \] (26)
which has the same leading behaviour for large \( z \) as \( zE_1(z) \). It also goes to zero for \( z \to 0 \), is positive for all \( z \in [0, \infty) \), and is smaller than \( zE_1(z) \) for all \( z \). Thus, replacing \( \psi(n) \) by
\[ \psi(n) + \frac{(-1)^n}{n(n+1)} \] (27)
gives an improved estimator. Apart from a misprint, this is the estimator recommended in \[ 4 \], Eq.(13).

This equation had been derived in \[ 4 \] somewhat unsystematically, using asymptotic series expansions in an uncontrolled way. Because of that, the discussion of the more general approximation, Eq.(11) in that paper, is wrong. In particular, Eq.(11) holds (for \( q \to 1 \)) not for all integer \( R \), but only for odd values of \( R \). Furthermore, the fact that the terms neglected in Eq.(11) decrease as \( z^{-R}e^{-z} \) for large \( z \) does not mean that Eq.(11) is exact in the limit \( R \to \infty \). Finally, in contrast to what is said there, this limit can be taken without a risk of statistical errors blowing up, at least for \( q \to 1 \).

Instead of following the derivation of \[ 4 \], we consider the semi-infinite sequence of real numbers \( G_1, G_2, \ldots \) defined by
\[ G_1 = -\gamma - \ln 2, \]
\[ G_2 = -\gamma - \ln 2, \]
\[ G_{2n+1} = G_{2n}, \] (28)
(here, \( \gamma = 0.577215 \ldots \) is Euler’s constant) and
\[ G_{2n+2} = G_{2n} + \frac{2}{2n+1} \quad (n \geq 1). \] (29)
Thus \( G_2n = -\gamma - \ln 2 + 2/1 + 2/3 + 2/5 + \ldots + 2/(2n-1) \).

Using the representation \( \psi(n) = -\gamma + 1/1 + 1/2 + 1/3 + \ldots + 1/(n-1) \), one checks that
\[ G_n = \psi(n) + (-1)^n \int_0^1 \frac{x^{n-1}}{x+1} dx. \] (30)

On the one hand, using formula 0.244 of \[ 16 \], one can write this integral as an infinite sum,
\[ G_n = \psi(n) + (-1)^n \sum_{l=0}^{\infty} \frac{1}{(n+2l)(n+2l+1)}, \] (31)
which can be compared to Eq.(11) of \[ 4 \] with \( q \to 1 \) and odd \( R \to \infty \). On the other hand, we obtain
\[ E[n(G_n - \psi(n))] = \sum_{n=1}^{\infty} n(G_n - \psi(n)) \frac{z^n}{n!} e^{-z} \]
\[ = - \int_0^1 dx \frac{e^{-z}}{x+1} \sum_{n=1}^{\infty} (-x)^{n-1} \]
\[ = -e^{-z} \int_0^1 dx \frac{e^{-xz}}{x+1} \]
\[ = -z(E_1(z) - E_1(2z)). \] (32)

Therefore, combining this with Eq.(21), we have
\[ E[nG_n] = z \ln z + zE_1(2z). \] (33)

This is our main result. Since the last term decreases as \( e^{-2z} \), the error made when neglecting it decreases exponentially faster with \( z = E[n] \) than when neglecting the last term in Eq.(21) for large \( z \). Thus, if all boxes have \( E[n_i] > 5 \), say, the error committed is \( < e^{-10} \) which should be negligible in all practical cases. More generally, the error made by neglecting the last term is again always negative, and it is bounded by
\[ 0 < -\Delta H_\psi < 0.1407 \ldots \times M/N, \] (34)
where \[ 14 \]
\[ \tilde{H}_\psi = \ln N - \frac{1}{N} \sum_{i=1}^{M} n_i G_n_i \] (35)
is our proposed best estimator.

Let us denote by \( z^* = 0.217 \ldots \) the position of the maximum of \( zE_1(2z) \). For \( z < z^* \) this function is convex. Thus, if \( N/M < z^* \), the distribution of \( z \)-values over the boxes which gives the maximal bias is a delta function, \( P(z) = \delta(z - N/M) \), and Eq.(34) can be improved to \( -\Delta H_\psi \leq E_1(2N/M) \).

For \( N/M \to 0 \) this diverges \( \sim \ln(M/N) \).

We might add that truncating the sum in Eq.(31) at any finite \( l \) also gives valid estimators whose errors are between those of \( \tilde{H}_G \) and \( \tilde{H}_\psi \), but there seems no reason to prefer any of them over \( \tilde{H}_G \) or \( \tilde{H}_\psi \). Taking only the term with \( l = 0 \) gives Eq.(27).

The error terms \( E[n\psi(n)] - z \ln z \) for \( \psi(n) = \ln n, \ln n - 1/2, \psi(n), \psi(n) + (-1)^n n/(n+1), \) and \( G_n \) are shown in Fig.1, together with one more curve discussed below. The functions \( \psi(n) \) themselves are shown in Fig.2.

We can give estimators with even smaller absolute bias, i.e., with \( |\Delta H| < 0.1407 \ldots \), but they have several drawbacks:
Their biases can have either sign.

We were only able to find them numerically, by minimizing (by simulated annealing) a cost function like e.g. the $L^2$ norm

$$
\delta = \int_0^\infty \frac{dz}{\sqrt{z}} \left| \sum_{n=1}^\infty n \phi(n) \frac{z^n}{n!} e^{-z} - z \ln z \right|^2.
$$

Typical results obtained in this way are shown in Figs. 1 and 2 [17].

- The resulting function $\phi(n)$ replacing $\psi(n)$ resp. $G_n$ is not monotonic, and its total variation as measured e.g. by $\sum_{n=1}^\infty n |\phi(n) - G_n|^2$ would diverge as $\delta \to 0$ (indeed, the results shown in Figs. 1 and 2 were obtained by adding 0.0002 times this term as a regularizer to the $L^2$ norm). This is the most serious drawback. It means that large cancellations must occur and thus statistical errors blow up in the limit $\delta \to 0$ (if $N$ is kept finite), as is to be expected on general grounds [3]. There cannot be any estimator of $H$ completely free of bias for finite $N$. Notice that $G_n$ is the "best" sequence which is still monotonic. Estimates based on non-monotonic $\phi(n)$ might be useful if one has important contributions from extremely small $z_i$, i.e. if either $N \ll M$ or if the distribution of $p_i$ is so uneven that many boxes have small (but not too small) $z_i$.

I have applied the above estimators to the six examples shown in Fig. 4 of [12]. In each of these examples the number of boxes was $M \geq 1000$, although the number of non-empty boxes was smaller in some of them. Nevertheless, the distributions were severely undersampled in most cases when $N \leq 300$. In all cases the annealed $\phi(n)$ shown in Fig. 2 gave statistical errors smaller or comparable to the Bayesian estimators of [12], and the bias was smaller than the statistical errors for all $N \geq 300$. In all but two cases (Zipf’s law and $\beta = 1$, with $\beta$ defined in [12]) the bias was negligible even down to $N = 10$. With Eq. (35), the bias was significant ($> 2\sigma$) in the same two cases for all $N \leq 300$, and in the case $\beta = 0.02$ for $N = 10$.

In summary, I hope to have clarified the arguments and corrected the mistakes made in [4], and I have substantially improved on the results. I have proposed a new analytic estimator for Shannon entropy which has very small systematic errors, except when the average number of points per box is much smaller than 1. Its statistical errors should be larger than those of the naive estimator (since there contributions from $n_i = 1$ and from $n_i > 1$ partially cancel), but this difference should be small. In addition, it is shown that numerically obtained estimators can be useful for extremely undersampled cases. The estimator $\hat{H}_p$ and the first correction based on Eq. (27) can be generalized straightforwardly to Renyi entropies, but I was not able to generalize the new estimator, Eq. (35), to $q \neq 1$. The present estimators cannot match the best Bayesian estimators [12] when the sampling is extremely low, but they are much simpler to use and more robust, as no guess of any prior distribution is needed.

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[1] G. Miller, Note on the bias of information estimates. In H. Quastler, ed., *Information theory in psychology II-B*, pp 95-100 (Free Press, Glencoe, IL 1955).
The last term can be estimated very similarly to the last term in Eq. (21), in particular it is positive and is bounded for all N and p by \( \frac{N}{N-1} (1-p) N \). In the estimator Eq. (23) which results from neglecting this term, replacing the Poisson distribution by the correct binomial one amounts to replacing \( \ln N \) by \( \psi(N) \) (brining e.g. Miller’s correction from \( M/2N \) down to \( (M-1)/2N \)). Similarly, in Eq. (25) one should replace \( \ln N \) by \( G_N \), in order to correct for the most important \( O(1/N) \) term not included in the Poisson approximation. For all estimators (including those where \( \phi(n) \) is obtained numerically), one should replace in Eq. (8) \( \ln N \) by \( \phi(N) \).

[15] M. Abramowitz and I. Stegun, eds., Handbook of Mathematical Functions (Dover, New York 1965).

[16] I.S. Gradshteyn and I.M. Ryshik, Tables of Integrals, Series, and Products (Academic Press, New York 1965).

[17] The coefficients \( \phi(n) \) for this solution can be obtained by sending an e-mail to p.grassberger@fz-juelich.de.