On Generalized Schüermann Entropy Estimators

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We present a new class of estimators of Shannon entropy for severely undersampled discrete distributions. It is based on a generalization of an estimator proposed by T. Schüermann, which itself is a generalization of an estimator proposed by myself in [arXiv:physics/0307138]. For a special set of parameters they are completely free of bias and have a finite variance, something which is widely believed to be impossible. We present also detailed numerical tests where we compare them with other recent estimators and with exact results, and point out a clash with Bayesian estimators for mutual information.

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 and eliminate this bias [1–22]. Some make quite strong assumptions [3–7], others use Bayesian methods [6–11, 12, 19, 21, 22]. As pointed out in [13, 14, 15, 17], 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. As conjectured in [13, 15, 17] the variance of any estimator whose bias vanishes will have a diverging variance.

Another widespread belief is that Bayesian entropy estimators cannot be outperformed by non-Bayesian ones for severely undersampled cases. The problem with Bayesian estimators is of course that they depend on a good choice of prior distributions, which is not always easy, and they tend to be slow. One positive feature of Bayesian estimators is of course that they depend on a good choice of prior distributions, which is not always easy, and they tend to be slow. One positive feature of Bayesian estimators is that they can be computed exactly. We will show that – even if $H$ cannot be estimated unambiguously. In that limit, the present algorithm seems to choose systematically a different outcome from Bayesian methods, for reasons that are not yet clear.

In the following we shall use the notation of [14]. As in this reference, we consider $M > 1$ “boxes” (states, possible experimental outcomes, ...) and $N > 1$ points (samples, events, particles) distributed randomly and independently into the boxes. We assume that each box has weight $p_i$ ($i = 1, \ldots, M$) with $\sum_i p_i = 1$. Thus each box $i$ will contain a random number $n_i$ of points, with $E[n_i] = p_iN$. Their joint distribution is multinomial,

$$P(n_1, n_2, \ldots, n_M; N) = N! \prod_{i=1}^{M} \frac{p_i^{n_i}}{n_i!},$$

while the marginal distribution in box $i$ is binomial,

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

Our aim is to estimate the entropy,

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

with $z_i = E[n_i] = p_iN$, 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 $H$,

$$\Delta[\hat{H}] \equiv E[\hat{H}] - H \neq 0,$$

as will also be its variance Var[$\hat{H}$]. Notice that for computing $E[\hat{H}]$ we need only Eq.(2), not the full multinomial
distribution of Eq.(1). But if we want to compute this variance, we need in addition the joint marginal distribution in two boxes,

\[ P(n_i, n_j; p_i, p_j, N) = \frac{N!}{n_i!n_j!(N - n_i - n_j)!} \times (5) \]

\[ p_i^n p_j^{n_j} (1 - p_i - p_j)^{N - n_i - n_j}, \]

in order to compute the covariances between different boxes. Notice that these covariances were not taken into account in [13, 17], whence the variance estimations in these papers are at best approximate.

In the following, we shall mostly be interested in the case of large but finite \( N \), where also the variance is positive, and we will discuss the balance between demanding minimal bias versus minimal variance.

Indeed it is well known that the naive (or ‘maximum-likelihood’) estimator, obtained by assuming \( z_i = n_i \) without fluctuations,

\[ \hat{H}_{\text{naive}} = \ln N - \frac{1}{N} \sum_{i=1}^{M} n_i \ln n_i, \]

(7)

is negatively biased, \( \Delta \hat{H}_{\text{naive}} < 0 \).

In order to estimate \( \hat{H} \), we have to estimate \( p_i \ln p_i \) or equivalently \( z_i \ln z_i \) for each \( i \). Since the distribution of \( n_i \) depends, according to Eq.(2), on \( z_i \) only, we can make the rather general ansatz \( 4, 14 \) for the estimator

\[ z_i \ln z_i = n_i \phi(n_i) \]

(8)

with a yet unknown function \( \phi(n) \). Notice that \( \hat{H} \) becomes with this ansatz a sum 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 \( 14 \)

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

(9)

with the overbar indicating an average over all boxes,

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

(10)

Its bias is

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

(11)

with

\[ \mathbb{E}_{N,z}[f_n] = \sum_{n=1}^{\infty} f_n P_{\text{binom}}(n; p = z/N, N). \]

(12)

being the expectation value for a typical box (in the following we shall suppress the box index \( i \) to simplify notation, wherever this makes sense).

In the following, \( \psi(x) = d \ln \Gamma(x)/dx \) is the digamma function, and

\[ E_1(x) = \Gamma(0, x) = \int_{1}^{\infty} e^{-xt} \frac{dt}{t} \]

(13)

is an exponential integral (Ref. [23], paragraph 5.1.4). It was shown in [14] that

\[ E_{N,z}[n \psi(n)] = z \ln z + \psi(N) - \ln N + z \int_{0}^{1-z/N} \frac{x^{N-1}dx}{1-x}, \]

(14)

which simplifies in the Poisson limit (\( N \rightarrow \infty \), \( z \) fixed) to

\[ E_{N,z}[n \psi(n)] \rightarrow z \ln z + z E_1(z). \]

(15)

Eqs.(14) and (15) will be the starting points of all further analysis. In [14] it was proposed to re-write Eq.(15) as

\[ E_{N,z}[nG_n] \rightarrow z \ln z + z E_1(2z), \]

(16)

where

\[ G_n = \psi(n) + (-1)^n \int_{0}^{1} \frac{x^{n-1}}{x+1} dx. \]

(17)

The advantages are that \( G_n \) can be evaluated very easily by recursion (here \( \gamma = 0.57721... \) is the Euler-Mascheroni constant), \( G_1 = G_2 = -\gamma - \ln 2 \), \( G_{2n+1} = G_{2n} \), and \( G_{2n+2} = G_{2n} + \frac{1}{2n+1} \), and neglecting the second term, \( z E_1(2z) \), gives an excellent approximation unless \( z \) is exceedingly small, i.e. unless the numbers of points per box are very small so that the distribution is very severely undersampled. Thus the entropy estimator proposed in [14] was simply

\[ \hat{H}_G = \ln N - \frac{1}{N} \sum_{i=1}^{M} n_i G_{n_i}. \]

(18)

Furthermore, since \( z E_1(2z) \) is positive definite, neglecting it gives a negative bias in \( \hat{H}_G \), and one can show rigorously that this bias is smaller than that of \( 11, 13 \).

The easiest way to understand the Schuermann class of estimators [15] is to define, instead of \( G_n \), a one-parameter family of functions

\[ G_a(a) = \psi(n) + (-1)^n \int_{0}^{a} \frac{x^{n-1}}{x+1} dx. \]

(19)
Notice that \( G_n(1) = G_n \) and \( G_n(0) = \psi(n) \).

Let us first discuss the somewhat easier Poissonian limit, where

\[
E_{N,z}[n(G_n(a) - \psi(n))] = \sum_{n=1}^{\infty} (-1)^n P_{\text{Poisson}}(n, z) \int_0^a \frac{x^{n-1}}{x+1} dx = -ze^{-z} \int_0^a \frac{dx}{x+1} e^{-xz} = -z(E_1(z) - E_1((1+a)z)),
\]

which gives

\[
E_{N,z}[nG_n(a)] = z \ln z + zE_1((1+a)z). \tag{20}
\]

Using \( a \) to achieve optimality \( a \) different parameters \( a_i \) for different boxes, and neglecting the right hand side of Eq.(20), we obtain finally

\[
\hat{H}_{\text{Schuermann}} = \ln N - \frac{1}{N} \sum_{i=1}^{M} n_i G_n(a_i) \quad \text{(Poissonian).} \tag{22}
\]

The reason why the r.h.s. of Eq.(20) can be neglected for sufficiently large \( a_i \) is simply that \( 0 < E_1(bz) < \exp(-bz) \) for any real \( b > 0 \).

For the general binomial case the algebra is a bit more involved. By somewhat tedious but straightforward algebra one finds that

\[
E_{N,z}[n(G_n(a) - \psi(n))] = \sum_{n=1}^{\infty} (-1)^n \frac{N}{n} p^n (1-p)^{N-n} \int_0^a \frac{x^{n-1}}{x+1} dx = -pN \int_0^a \frac{dx}{x+1} \sum_{n=1}^{\infty} \left(1-p\right)^{n-1}(1-p)^{N-n} = -pN \int_0^a \frac{dx}{x+1} (1-p - x) \left(1-p - \frac{x}{N}\right)^{N-1}.
\]

One immediately checks that this reduces, in the limit \( N \to \infty \), \( z \) fixed, to Eq.(20). On the other hand, by substituting

\[
x \to t = 1 - \frac{(1+x)z}{N}, \tag{24}
\]

in the integral, we obtain

\[
E_{N,z}[n(G_n(a) - \psi(n))] = -z \int_{1 - (1+a)z/N}^{1-z/N} \frac{t^{N-1}dt}{1-t}. \tag{25}
\]

Finally, by combining with Eq.(14), we find \([15]\)

\[
E_{N,z}[n(G_n(a))] = z \ln z + z[\psi(N) - \ln N] + z \int_0^{1-(1+a)z/N} \frac{x^{N-1}dx}{1-x} \tag{26}
\]

and

\[
\hat{H}_{\text{opt}} = \psi(N) - \frac{1}{N} \sum_{i=1}^{M} n_i G_n(a_i), \quad \text{(binomial)} \tag{27}
\]

with a correction term whose bias vanishes when the integration range on the r.h.s. of Eq.(20) is zero. Notice that we use here, in general, a different parameter \( a_i \) for each box \( i \). In \([15]\) one single parameter \( a \) was used, which is why we call our method a generalized Schuermann estimator.

This is a remarkable result, as it shows that the analytic correction to the naive estimator, as given by Eqs.(19) and (27), become exact when for each box \( i \)

\[
a_i \to a_i^* \equiv \frac{1 - p_i}{p_i}. \tag{28}
\]

When all box weights are small, \( p_i \ll 1 \) for all \( i \), then these bias-optimal values of \( a_i \) are very large. But for two boxes with \( p_1 = p_2 = 1/2 \), e.g., the bias vanishes already for \( a_1 = a_2 = 1 \), i.e. for the estimator of Grassberger \([13]\).

In order to test the latter, we drew \( 10^8 \) triplets of random bits (i.e., \( N = 3 \), \( p_0 = p_1 = 1/2 \)), and estimated \( \hat{H}_{\text{naive}} \) and \( \hat{H}_G \) for each triplet. From these we computed averages and variances, with the results \( \hat{H}_{\text{naive}} = 0.68867(4) \) bits and \( \hat{H}_G = 0.99995(4) \) bits. We should stress that the latter requires the precise form of Eq.(27) to be used, with \( \psi(N) \) neither replaced by \( \ln N \) nor by \( G_N \).

Since there is no free lunch, there must of course be some problems in the limit when parameters \( a_i \) are chosen nearly bias-optimal. One problem is that one cannot, in general, choose \( a_i \) according to Eq.(28), because the \( p_i \) are unknown. In addition, it is in this limit (and more generally when \( a_i >> 1 \)) that variances blow up. In order to see this, we have to discuss in more detail the properties of the functions \( G_n(a) \).

According to Eq.(19), \( G_n(a) \) is a sum of two terms, both of which can be computed, for all positive integer \( n \), by recursion. The digamma function \( \psi(n) \) satisfies

\[
\psi(1) = -\gamma, \quad \psi(n+1) = \psi(n) + 1/n. \tag{29}
\]

Let us denote the integral in Eq.(19) as \( g_n(a) \). It satisfies the recursion

\[
g_1(a) = -\ln(1+a), \quad g_{n+1}(a) = g_n(a) + (-a)^n/n. \tag{30}
\]

Thus, while \( \psi(n) \) is monotonic and slowly increasing, \( g_n(a) \) has alternating sign and increases, for \( a > 1 \), exponentially with \( n \). As a consequence, also \( G_n(a) \) is non-monotonic and diverges exponentially with \( n \), whenever \( a > 1 \). Therefore an estimator like \( \hat{H}_{\text{opt}} \) gets, unless all \( n_i \) are very small, increasingly large contributions of alternating signs. As a result variances will blow up, unless one is very careful to keep a balance between bias and variance.
FIG. 1: Estimated entropies (in bits) of N-tuples of i.i.d. random binary variables with \( p_0 = 0.625 \) and \( p_1 = 0.25 \), using the optimized estimator \( H_{\text{opt}} \), defined in Eq. (27). The parameter \( a_0 \) was kept fixed at its optimal value \( a_0 = 1/3 \), while \( a_1 \) was varied in view of possible problems with the variances, and is plotted on the horizontal axis. For each \( N \) and each value of \( a_1 \), \( 10^8 \) tuples were drawn. The exact entropy for \( p_0 = 3/4 \) and \( p_1 = 1/4 \) is 0.811278... bits, and is indicated by the horizontal straight line.

FIG. 2: Estimated entropies (in bits) of N-tuples of i.i.d. random ternary variables with \( p_0 = 0.625 \), \( p_1 = 0.25 \), and \( p_2 = 0.125 \), using the optimized estimator \( H_{\text{opt}} \), defined in Eq. (27). The parameter \( a_0 \) was kept fixed at its optimal value \( a_0 = 1/3 \), while \( a_1 \) and \( a_2 \) varied in view of possible problems with the variances. More precisely, we used \( a_2 = 1 + 4(a_1 - 1) \), so that the data end at the bias-free values \( a_1^* = 2.5 \) and \( a_2^* = 7.0 \). For each \( N \) and each value of \( a_1 \), \( 10^8 \) tuples were drawn. The exact entropy is 1.29879... bits, and is indicated by the horizontal straight line.

To illustrate this we drew tuples of i.i.d. binary variables \( \{s_1,...,s_N\} \) with \( p_0 = 3/4 \) and \( p_1 = 1/4 \). For \( a_0 \) we chose \( a_0 = a_1^* = 1/3 \), because this should minimize the bias and should not create problems with the variance. We should expect such problems, however, if we would take \( a_1 = a_1^* = 3 \), although this would reduce the bias to zero. Indeed we found for \( N = 100 \) that the variance of the estimator exploded for all practical purposes as soon as \( a_1 > 1.4 \), while the results were optimal for \( 0.5 < a_1 \leq 1 \) (bias and statistical error were both \( < 10^{-5} \) for \( 10^8 \) tuples). On the other hand, for pairs (\( N = 2 \)) we had to use much larger values of \( a_1 \) for optimality, and \( a_1 = 3 \) gave indeed the best results (see Fig.1). A similar plot for ternary variables is shown in Fig.2, where we see again that the bias-optimal values gave estimates with zero bias and acceptable variance for the most undersampled case \( N = 2 \).

The message to be learned from this is that we should always keep all \( a_i \) sufficiently small that \( a_i^{n_i} \leq O(1) \) for the observed values of \( n_i \).

Finally, we apply our estimator to two problems of mutual information (MI) estimation discussed in [22] (actually, the problems were originally proposed by previous authors, but we shall compare our results mainly to those in [22]. In each of these problems there are two discrete random variables: \( X \) has many (several thousand) possible values, while \( Y \) is binary. Moreover, the marginal distribution of \( Y \) is uniform, \( p(y = 0) = p(y = 1) = 1/2 \), while the \( X \)-distributions are highly non-uniform. Finally – and that is crucial – the joint distributions show no obvious regularities.

The MI is estimated as \( I(X : Y) = H(Y) - H(Y|X) \). Since \( H(Y) = 1 \) bit, the problem essentially burns down to estimate the conditional probabilities \( p(y|x) \). The data are given in terms of a large number of i.i.d. sampled pairs \((x,y)\) (250,000 pairs for problem I, called ‘PYM’ in the following, and 50,000 pairs for problem II, called ‘spherical’ in the following). The task is to draw random subsamples of size \( N \), to estimate the MI from each subsample, and to calculate averages and statistical widths from these estimates.

Results are shown in Fig. 3. For large \( N \) our data agree perfectly with those in [22] and in the previous papers cited in [22]. But while the MI estimates in these previous papers all increase with decreasing \( N \), and those in [22] stay essentially constant (as we would expect, since a good entropy estimator should not depend on \( N \), and conditional entropies should decrease with \( N \) for not so good estimators), our estimated MI decreases to zero for small \( N \).

This looks at first sight like a failure of our method, but it is not. As we said, the joint distributions show no regularities. For small \( N \) most values of \( X \) will show up at most once, and if we write the sequence of \( y \)-values in a typical tuple, it will look like a perfectly random binary string. The modeler knows that it actually is not random, because there are correlations between \( X \) and \( Y \). But no algorithm can know this, and any good algorithm should conclude that \( H(Y|X) = H(Y) = 1 \) bit. Why, then was this not found in the previous analyses? In all these, Bayesian estimators were used. If the priors used in these estimators were chosen in view of the special structures in the data (which are, as we should stress again, not visible from the data, as long as these are severely undersampled!), then the algorithms can make...
Thus each $x$ value is realized $\approx 60$ times, and we classify them into 5 classes depending on the associated $y$-values: (i) very heavily biased towards $y = 1$, (ii) moderately biased towards $y = 1$, (iii) $y$-neutral, (iv) moderately biased towards $y = 0$, and (v) heavily biased towards $y = 0$. When we estimated conditional entropies $H(Y|X)$ for randomly drawn subsamples, we kept this classification and choose $a_y$ accordingly: For class (iii) we used $a_0 = a_1 = 1$, for class (ii) we used $a_1 = 1, a_0 = 4$, for class (i) we used $a_1 = 1, a_0 = 7$, for class (iv) we used $a_1 = 4, a_0 = 1$, and finally for class (v) we used $a_1 = 7, a_0 = 1$. The data for "spherical", originally due to [21], consist of 50,000 $(x, y)$ pairs. Here, $Y$ is again binary with $p(y = 0) = p(y = 1) = 1/2$, but $X$ is highly non-uniformly distributed over $4000$ values. Again we classified these values as $y$-neutral or heavily / moderately biased towards or against $y = 0$ and used this classification to choose values of $a_y$ accordingly.

Finally, we pointed out that Bayesian methods which have been very popular in this field have the danger of choosing "too good" priors, i.e. choosing priors which are not justified by the data themselves and are thus misleading, although both the bias and the observed variances seem to be small.

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