A Better Good-Turing Estimator for Sequence Probabilities

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Abstract—We consider the problem of estimating the probability of an observed string drawn i.i.d. from an unknown distribution. The key feature of our study is that the length of the observed string is assumed to be of the same order as the size of the underlying alphabet. In this setting, many letters are unseen and the empirical distribution tends to overestimate the probability of the observed letters. To overcome this problem, the traditional approach to probability estimation is to use the classical Good-Turing estimator. We introduce a natural scaling model and use it to show that the Good-Turing sequence probability estimator is not consistent. We then introduce a novel sequence probability estimator that is indeed consistent under the natural scaling model.

I. INTRODUCTION

Suppose we are given a string drawn i.i.d. from an unknown distribution. Our goal is to estimate the probability of the observed string. One approach to this problem is to use the type, or empirical distribution, of the string as an approximation of the true underlying distribution and then to calculate the resulting probability of the observed string. It is well known that this estimator assigns to each string its largest possible probability under an i.i.d. distribution. For large enough observation sizes, this estimator works well; indeed, for large $n$ and a fixed underlying distribution, it is a consistent sequence probability estimator.

Motivated by applications in natural language, we focus on a nonstandard regime in which the size of the underlying alphabet is of the same order as the length of the observed string. In this regime, the type of the observation is a poor representation of the true probability distribution. Indeed, many letters with nonzero probability will not be observed at all and the type will obviously assign these letters zero probability. This would not make for a consistent probability estimator.

Since probability estimation and compression are closely related, we can turn to the compression literature for succor. The results in this literature are negative, however. For instance, Orlitsky and Santhanam [1] shows that universal compression of i.i.d. strings drawn from an alphabet that grows linearly with the observation size is impossible. As such, the compression literature is unhelpful and even suggests that seeking a consistent universal sequence probability estimator might be futile.

Nevertheless, sequence probability estimation is of such importance in applications that several heuristic approaches have been developed. The foremost among them is based on the classical Good-Turing probability estimator (see Section IV). The idea is to use the Good-Turing estimator instead of the type to estimate the underlying probability distribution. The probability of the sequence can then be calculated accordingly. Orlitsky et al. [3] have studied the performance of a similar scheme in the context of probability estimation for patterns. No theoretical results regarding the performance of this approach for sequence probability estimation are available, however.

To analyze the performance of this scheme, we introduce a natural scaling model in which the number of observations, $n$, and the underlying alphabet size grow at the same rate. Further, the underlying probabilities vary with $n$. The only restriction we make is that no letter should be either too rare or too frequent. That is, the probability that any given symbol occurs somewhere in the string should be bounded away from 0 and 1 as the length of the string tends to infinity. In particular, this condition requires that the probabilities of the letters be $\Theta(1/n)$. We call this the rare events regime. This scaling model is formally described in the next section.

Our model is similar to the one used by Klaassen and Mnatsakanov [4] and Khmaladze and Chitashvili [5] to study related problems. We used this model previously [6] to show consistency of the Good-Turing estimate of the total probability of letters that occur a given number of times in the observed string. In the present paper, we use this model to first show that the Good-Turing estimator for sequence probabilities performs poorly; in fact, a simple example illustrates that it is not consistent. Drawing from this example, we then provide a novel sequence probability estimator that improves upon the Good-Turing estimator—in fact, we show that it is consistent in the context of the natural scaling model. This is done in Section V. Finally, we discuss the application of our results to universal hypothesis testing problems in the rare event regime in Section VI.
II. THE RARE EVENTS REGIME

Let $\Omega_n$ be a sequence of finite alphabets. For each $n$, let $p_n$ and $q_n$ be probability measures on $\Omega_n$ satisfying

$$\hat{c} \leq \min(p_n(\omega), q_n(\omega)) \leq \max(p_n(\omega), q_n(\omega)) \leq \hat{c}$$  \hspace{1cm} (1)

for all $\omega \in \Omega_n$, where $\hat{c}$ and $\hat{c}$ are fixed constants that are independent of $n$. Observe that this requires the cardinality of the alphabet size to grow linearly in $n$

$$\frac{n}{\hat{c}} \leq |\Omega_n| \leq \frac{n}{\hat{c}}$$

We observe two strings of length $n$. The first, denoted by $x$, is a sequence of symbols drawn i.i.d. from $\Omega_n$ according to $p_n$. The second, denoted by $y$, is a sequence of symbols drawn i.i.d. from $\Omega_n$ according to $q_n$. We assume that $x$ and $y$ are statistically independent. Note that both the alphabet and the underlying probability measures are permitted to vary with $n$. Note also that by assumption (1), each element of $\Omega_n$ has probability $\Theta(1/n)$ under both measures and thus will appear $\Theta(1)$ times on average in both strings. In fact, the probability of a given symbol appearing a fixed number of times in either string is bounded away from 0 and 1 as $n \to \infty$. In other words, every letter is rare. The number of distinct symbols in either string will grow linearly with $n$ as a result.

Our focus shall be on the quantities $p_n(x)$ and $p_n(y)$. An important initial observation to make is that the distributions of these two random variables are invariant under a relabeling of the elements of $\Omega_n$. It is therefore convenient to consider the probabilities assigned by the measures $p_n$ and $q_n$ without reference to the labeling of the symbols. It is also convenient to normalize these probabilities so that they are $\Theta(1)$.

Let $P_n$ denote the distribution of

$$(p_n(x_n), q_n(x_n)),$$

where $x_n$ is drawn according to $p_n$. Likewise, let $Q_n$ denote the distribution of

$$(p_n(y_n), q_n(y_n)),$$

where $y_n$ is drawn according to $q_n$.

Note that both $P_n$ and $Q_n$ are probability measures on $C := [\hat{c}, \hat{c}] \times [\hat{c}, \hat{c}]$. It follows from the definitions that $P_n$ and $Q_n$ are absolutely continuous with respect to each other and the Radon-Nikodym derivative is given by

$$\frac{dQ_n}{dP_n}(x, y) = \frac{y}{x}.$$  \hspace{1cm} (2)

Note that many quantities of interest involving $p_n$ and $q_n$ can be computed using $P_n$ (or $Q_n$). For example, the entropy of $p_n$ can be expressed as

$$-\int_C \log\frac{x}{n} dP_n(x, y)$$

and the relative entropy between $p_n$ and $q_n$ is given by

$$D(p_n|q_n) = \int_C \log\frac{x}{y} dP_n(x, y).$$

We shall assume that $P_n$ converges in distribution to a probability measure $P$ on $C$. Since $P_n$ and $Q_n$ are related by (2), this implies that $Q_n$ converges to a distribution $Q$ satisfying

$$\frac{dQ}{dP}(x, y) = \frac{y}{x}.$$  \hspace{1cm} (3)

III. PROBLEM FORMULATION

Recall that the classical (finite-alphabet, fixed-distribution) asymptotic equipartition property (AEP) asserts that

$$\lim_{n\to\infty} \frac{1}{n} \log \mu(w) = -H(\mu) \text{ a.s.,}$$

where $w$ is an i.i.d. sequence drawn according to $\mu$ and $H(\cdot)$ denotes discrete entropy. Loosely speaking, (3) says that the probability of the observed sequence, $\mu(w)$, is approximately

$$\exp(-nH(\mu)),$$

In the rare events regime, on the other hand, one expects the probability of an observed sequence to be approximately

$$\left(\frac{h}{n}\right)^n$$

for some constant $h$. Indeed, in the rare events regime the following AEP holds true (all proofs are contained in Section VII).

**Theorem 1:**

$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^n \log(p_n(x_i)) = \int_C \log(x) dP(x, y) \text{ a.s.}$$

Our goal is to estimate the limit in Theorem 1 universally, that is, using only the observed sequence $x$ without reference to the probability measures $p_n$. Of course, in the classical setup, the analogous problem of universally estimating the limit in (3) is straightforward. The distribution $\mu$ can be determined from the observed sequence by the law of large numbers, from which the entropy $H(\mu)$ can be calculated. In the rare events regime, on the other hand, this approach fails and the problem is more challenging.

We shall also study the following variation on this problem. Consider the related quantity $p_n(y)$. That is, the sequence is generated i.i.d. according to $q_n$, but we evaluate its probability under $p_n$. This quantity arises in detection problems, where one must determine the likelihood of a given realization under multiple probability distributions. As in the single-sequence setup, it turns out that this probability converges if it is suitably normalized.

**Theorem 2:**

$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^n \log(p_n(y_i)) = \int_C \log(x) dQ(x, y) \text{ a.s.}$$

Our goal is then to estimate the limit in Theorem 2 using only the observed sequences $x$ and $y$. Again, in a fixed-distribution setup, this problem is straightforward because the two distributions can be determined exactly from the observed sequences in the limit as $n$ tends to infinity. In the rare events regime, however, the problem is more challenging.
IV. THE GOOD-TURING ESTIMATOR

The Good-Turing estimator can be viewed as an estimator for the probabilities of the individual symbols. Let \( A_k \) be the set of symbols that appear \( k \) times in the sequence \( x \), and let \( \varphi_k = |A_k| \) denote the number of such symbols. The basic form of the Good-Turing estimator assigns probability

\[
\frac{(k+1)\varphi_{k+1}}{n\varphi_k}
\]

(4)

to each symbol that appears \( k \leq n-1 \) times [2]. The case \( k = n \) must be handled separately, but this case is unimportant to us because in the rare events regime the chance that only one symbol appears in \( x \) is asymptotically negligible.

The Good-Turing formula can also be viewed as an estimator for the total probability of all symbols that appear \( k \) times in \( x \), i.e., \( p_n(A_k) \). In particular, the \( \varphi_k \) in the denominator can be viewed as simply dividing the total probability

\[
\frac{(k+1)\varphi_{k+1}}{n}
\]

equally among the \( \varphi_k \) symbols that appear \( k \) times. In previous work, we showed that the Good-Turing total probability estimator is strongly consistent in that for any \( k \geq 0 \),

\[
\lim_{n \to \infty} \frac{(k+1)\varphi_{k+1}}{n} = \lim_{n \to \infty} p_n(A_k) = \int C \frac{x^k e^{-x}}{k!} \, dP(x, y) =: \lambda_k \quad \text{a.s.} \quad (5)
\]

(see [6], where the notation is slightly different, for a proof of a stronger version of this statement). The Good-Turing probability estimator in (4) gives rise to a natural estimator for the probability of the observed sequence \( x \)

\[
\prod_{k=1}^{n-1} \left( \frac{(k+1)\varphi_{k+1}}{n\varphi_k} \right)^{k\varphi_k}.
\]

This in turn suggests the following estimator for the limit in Theorem I

\[
\sum_{k=1}^{n-1} \frac{k\varphi_k}{n} \log \left( \frac{(k+1)\varphi_{k+1}}{\varphi_k} \right). \quad (6)
\]

This estimator is problematic, however, because for the largest \( k \) for which \( \varphi_k > 0 \),

\[
\frac{(k+1)\varphi_{k+1}}{\varphi_k} = 0,
\]

which means that the \( k \)th term in (6) equals \( -\infty \). Various “smoothing” techniques have been introduced to address related problems with the estimator [2]. Our approach will be to truncate the summation at a large but fixed threshold, \( K \)

\[
\sum_{k=1}^{K} \frac{k\varphi_k}{n} \log \left( \frac{(k+1)\varphi_{k+1}}{\varphi_k} \right).
\]

In the rare events regime, with probability one it will eventually happen that \( \varphi_k > 0 \) for all \( k = 1, \ldots, K \), thus obviating the problem. By the result in (5), this estimator will converge to

\[
\sum_{k=1}^{K} \lambda_{k-1} \log \frac{k\lambda_k}{\lambda_{k-1}}. \quad (7)
\]

We next show that this quantity need not tend to the limit in Theorem I as \( K \) tends to infinity.

Let \( \Omega_n \) be the set \( \{1, 2, \ldots, 3n\} \). Suppose that \( p_n \) assigns probability \( 1/(4n) \) to the first \( 2n \) elements and probability \( 1/(2n) \) to the remaining \( n \). The distribution \( q_n \) is obviously not relevant here so we shall simply set it equal to \( p_n \).

The resulting distribution \( P \) will place mass \( 1/2 \) on each of the points \( (1/4, 1/4) \) and \( (1/2, 1/2) \). From Theorem I the limiting normalized probability of \( x \) is \( -(1/2) \log 8 \). By (7), the Good-Turing estimate converges to

\[
\frac{1}{2} \sum_{k=1}^{K} e^{-1/4}(1/4)^{k-1} \left( 1 + e^{-1/4}2^{k-1} \right) \cdot \log \left( \frac{\sqrt{8}(1 + e^{-1/4}2^k)}{4(1 + e^{-1/4}2^{k-1})} \right) + \frac{1}{2} \sum_{k=1}^{K} e^{-1/4}(1/4)^{k-1} \left( 1 + e^{-1/4}2^{k-1} \right) \log \frac{1}{\sqrt{8}}.
\]

Now as \( K \) tends to infinity, the second sum converges to the correct answer, \( -(1/2) \log 8 \). But one can verify that every term in the first sum is strictly positive. Thus the Good-Turing estimator is not consistent in this example.

The problem is that the Good-Turing estimator is estimating the sum, or equivalently the arithmetic mean, of the probabilities of the symbols appearing \( k \) times in \( x \). Estimating the sequence probability, on the other hand, amounts to estimating the geometric mean of these probabilities. If \( p_n \) assigns the same probability to every symbol, then the arithmetic and geometric means coincide, and one can show that the Good-Turing sequence probability estimator is asymptotically correct. In the above example, however, \( p_n \) is not uniform, and the Good-Turing formula converges to the wrong value. In the next section, we describe an estimator that targets the geometric mean of the probabilities instead of the arithmetic mean, and thereby correctly estimates the sequence probability.

V. A BETTER GOOD-TURING ESTIMATOR

Write

\[
\varpi = \frac{\hat{c} + \check{c}}{2},
\]

and then let

\[
\gamma^M_k = -\sum_{m=1}^{M} \sum_{\ell=0}^{m} (-1)^{-\ell} \left( \frac{m + \ell)!}{m \cdot \ell!} \frac{(k + \ell)! (k + \ell + 1)\varphi_{k+\ell+1}}{n} + \log(\varpi) (k+1)\varphi_{k+1} \right).
\]

Note that \( \gamma^M_k \) is only a function of \( x \) and in particular, it does not depend on \( p_n \). The next theorem shows that for large
is a consistent estimator for the limit in Theorem 1

Theorem 3: For any \( \epsilon > 0 \),

\[
\lim_{n \to \infty} \left| \frac{1}{n} \sum_{i=1}^{n} \log(np_n(x_i)) - \sum_{k=0}^{K} \gamma_k \right| \leq \epsilon \quad \text{a.s.} \quad (8)
\]

provided

\[
\max \left( \frac{\exp(\hat{c})}{\hat{c}} \left( \frac{\hat{c} - \hat{c}}{\hat{c} + \hat{c}} \right)^{M+1} \right) \leq \frac{\epsilon}{2},
\]

where

\[
c = \max(\log \hat{c}, \log \hat{d}).
\]

The idea behind Theorem 3 is this. Recall from (5) that

\[
\lim_{n \to \infty} \frac{(k+1)\varphi_{k+1}}{n} = \int_{C} x^k \exp(-x) \, dP(x, y) \quad \text{a.s.}
\]

If one could find a sequence of constants \( a_k \) such that

\[
\sum_{k=0}^{\infty} a_k \frac{x^k}{k!} = \log(x)
\]

on \([\hat{c}, \hat{d}]\), then one might expect that

\[
\lim_{n \to \infty} \sum_{k=0}^{n-1} a_k \frac{(k+1)\varphi_{k+1}}{n} = \int_{C} \log(x) \, dP(x, y) \quad \text{a.s.}
\]

This is indeed the approach we took to find the formula for \( \gamma_k^M \).

The estimator can be naturally extended to the two-sequence setup, namely to the problem of universally estimating \( p_n(y) \).

Let \( \varphi_{k,t} \) be the number of symbols in \( \Omega_n \) that appear \( k \) times in \( x \) and \( \ell \) times in \( y \). Then let

\[
\tilde{\gamma}_k^M = -\sum_{m=1}^{M} \sum_{\ell=0}^{(m-1)\ell} \binom{m}{\ell} \frac{(k+\ell)!}{m \cdot k!} \sum_{j=1}^{n} \frac{j \varphi_{k+\ell,j}}{n} + \log(n) \sum_{j=1}^{n} \frac{j \varphi_{k,j}}{n}.
\]

Note that \( \tilde{\gamma}_k^M \) is a function of \( x \) and \( y \).

Theorem 4: For any \( \epsilon > 0 \),

\[
\lim_{n \to \infty} \left| \frac{1}{n} \sum_{i=1}^{n} \log(np_n(y_i)) - \sum_{k=0}^{K} \tilde{\gamma}_k \right| \leq \epsilon \quad \text{a.s.}
\]

provided

\[
\max \left( \frac{\exp(\hat{c})}{\hat{c}} \left( \frac{\hat{c} - \hat{c}}{\hat{c} + \hat{c}} \right)^{M+1} \right) \leq \frac{\epsilon}{2},
\]

This result shows that although we are unable to determine \( p_n \) from \( x \), we are able to glean enough information about \( p_n \) to determine the limit in Theorem 2.

VI. Universal Hypothesis Testing

The \( \hat{\gamma}_k^M \) estimator leads to a natural scheme for the problem of universal hypothesis testing. Suppose that we again observe the sequences \( x \) and \( y \), which we now view as training data. In addition, we observe a test sequence, say \( z \), which is generated i.i.d. from the distribution \( r_n \). We assume that either \( r_n = p_n \) for all \( n \) or \( r_n = q_n \) for all \( n \). The problem is to determine which of these two possibilities is in effect using only the sequences \( x \), \( y \), and \( z \).

Using Theorem 4, one can estimate \( p_n(z) \) and \( q_n(z) \), and by comparing the two, determine which of the two distributions generated \( z \). This will make for a consistent universal classifier, without recourse to actually estimating the true underlying distributions \( p_n \) and \( q_n \). As a scheme for universal hypothesis testing, however, this approach is quite complicated and there is no reason to believe it would be optimal in an error-exponent sense. We are currently investigating other, more direct approaches to the universal hypothesis testing problem in the rare events regime. For a discussion of universal hypothesis testing in the traditional, fixed-distribution regime, see Gutman [7] and Ziv [8].

VII. Proofs

Due to space limitations, we will only prove Theorem 1 and sketch the proof of Theorem 3. The proofs of Theorems 2 and 4 are similar.

Lemma 1:

\[
\lim_{n \to \infty} E \left[ \frac{1}{n} \sum_{i=1}^{n} \log(np_n(x_i)) \right] = \int_{C} \log(x) \, dP(x, y).
\]

Proof: Note that for any \( i \)

\[
E[\log(np_n(x_i))] = \sum_{\omega \in \Omega_n} p_n(\omega) \log(np_n(\omega))
\]

\[
= \int_{C} \log(x) \, dP_n(x, y).
\]

Since \( \log(x) \) is bounded and continuous over \( C \) and \( P_n \) converges in distribution to \( P \), the result follows. \( \square \)

Lemma 2:

\[
\lim_{n \to \infty} \left| \frac{1}{n} \sum_{i=1}^{n} \log(np_n(x_i)) \right| - E \left[ \frac{1}{n} \sum_{i=1}^{n} \log(np_n(x_i)) \right] = 0 \quad \text{a.s.}
\]

Proof: Consider the sum

\[
\sum_{i=1}^{n} \log(np_n(x_i)).
\]

If one symbol in the sequence \( x \) is altered, then this sum can change by at most

\[
\log(\hat{c}).
\]
It follows from the Azuma-Hoeffding-Bennett concentration inequality [9, Corollary 2.4.14] that
\[
\Pr \left( \left| \frac{1}{n} \sum_{i=1}^{n} \log(np_n(x_i)) - E \left[ \frac{1}{n} \sum_{i=1}^{n} \log(np_n(x_i)) \right] \right| > \epsilon \right) \leq 2 \exp \left( -\frac{c^n}{2(\log(\epsilon/c))^2} \right).
\]

The result then follows by the Borel-Cantelli lemma.

Note that Theorem 1 follows immediately from Lemmas 1 and 2.

The key step in the proof of Theorem 3 is showing that \( \gamma_k^M \) converges to the proper limit. This is shown in the next and final lemma.

**Lemma 3:** For any \( \epsilon > 0 \) and any \( k \geq 0 \),
\[
\lim_{n \to \infty} \left| \gamma_k^M - \int_C \log(x) \frac{\exp(-x)x^k}{k!} dP(x, y) \right| \leq \epsilon k \frac{\tau}{c} \frac{c - \bar{c}}{c + \bar{c}}^{M+1} \text{ a.s.},
\]
provided
\[
\frac{\tau}{c} \frac{c - \bar{c}}{c + \bar{c}}^{M+1} \leq \epsilon.
\]

**Proof (sketch):** Note that the limit exists by (5). By the triangle inequality,
\[
\left| \gamma_k^M - \int_C \log(x) \frac{\exp(-x)x^k}{k!} dP(x, y) \right| \leq \left| \gamma_k^M - \tau_k^M \right| + \left| \tau_k^M - \int_C \log(x) \frac{\exp(-x)x^k}{k!} dP(x, y) \right|,
\]
(9)
where
\[
\tau_k^M = \sum_{m=1}^{M} \sum_{\ell=0}^{m} (-\tau)^{-\ell} \binom{m}{\ell} \frac{(k + \ell)!}{m \cdot k!} \lambda_{k+\ell} + \log(\tau) \lambda_k.
\]
(10)
The first term on the right-hand side of (9) tends to zero by (5).

Now
\[
- \sum_{m=1}^{M} \sum_{\ell=0}^{m} (-\tau)^{-\ell} \binom{m}{\ell} \frac{(k + \ell)!}{m \cdot k!} \lambda_{k+\ell}
= - \int_C \sum_{m=1}^{M} \frac{\exp(-x)x^k}{m \cdot k!} (-\tau)^{-m}
\cdot \sum_{\ell=0}^{m} \binom{m}{\ell} (-\tau)^{m-\ell} x^\ell dP(x, y).
\]
By the Binomial Theorem,
\[
\sum_{\ell=0}^{m} \binom{m}{\ell} (-\tau)^{m-\ell} x^\ell = (x - \tau)^m.
\]
Substituting these last two equations into (10) yields
\[
\tau_k^M = - \int_C \sum_{m=1}^{M} \left( 1 - \frac{x}{\tau} \right)^m \frac{\exp(-x)x^k}{m \cdot k!} dP(x, y)
+ \log(\tau) \lambda_k.
\]

Using the well-known power series
\[
\log(1 + x) = \sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{m+1} x^m,
\]
valid for \(-1 < x \leq 1\), one can show that
\[
\sup_{\epsilon \leq x \leq \epsilon} \left| \log \frac{x}{\epsilon} + \sum_{m=1}^{M} \frac{1}{m} \left( 1 - \frac{x}{\epsilon} \right)^m \right| \leq \frac{\tau}{c} \frac{c - \bar{c}}{c + \bar{c}}^{M+1} \leq \epsilon
\]
by hypothesis. Thus
\[
\left| \tau_k^M - \int_C \log(x) \frac{\exp(-x)x^k}{k!} dP(x, y) \right|
= \left| \int_C \sum_{m=1}^{M} \left( 1 - \frac{x}{\tau} \right)^m \frac{\exp(-x)x^k}{m \cdot k!} dP(x, y) \right|
+ \left| \int_C \log \left( \frac{x}{\tau} \right) \frac{\exp(-x)x^k}{k!} dP(x, y) \right|
\leq \int_C \epsilon \frac{\exp(-x)x^k}{k!} dP(x, y) \leq \epsilon k \frac{\tau}{c} \frac{c - \bar{c}}{c + \bar{c}}^{M+1}.
\]

Since
\[
\sum_{k=0}^{\infty} \frac{\exp(-x)x^k}{k!} = 1,
\]
one would expect from Lemma 3 that for large \( K \) and \( M \),
\[
\sum_{k=0}^{K} \gamma_k^M
\]
would be close to
\[
\int_C \log(x) dP(x, y).
\]
Indeed, one can prove Theorem 3 using this approach. The details are omitted.

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