Bounds for Learning Lossless Source Coding

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Abstract

This paper asks a basic question: how much training is required to beat a universal source coder? Traditionally, there have been two types of source coders: fixed, optimum coders such as Huffman coders; and universal source coders, such as Lempel-Ziv. The paper considers a third type of source coders: learned coders. These are coders that are trained on data of a particular type, and then used to encode new data of that type. This is a type of coder that has recently become very popular for (lossy) image and video coding.

The paper considers two criteria for performance of learned coders: the average performance over training data, and a guaranteed performance over all training except for some error probability \( P_e \). In both cases the coders are evaluated with respect to redundancy.

The paper considers the IID binary case and binary Markov chains. In both cases it is shown that the amount of training data required is very moderate: to code sequences of length \( l \) the amount of training data required to beat a universal source coder is \( m = K \frac{l}{\log l} \), where the constant in front depends the case considered.

I. Introduction

Traditionally, there have been two types of source coders: fixed, optimum coders such as Huffman coders; and universal source coders, such as Lempel-Ziv [1], [2], [3]. We will consider a third type of source coders: learned coders. These are coders that are trained on data of a particular type, and then used to encode new data of that type. Examples could be source coders for English texts, DNA data, or protein data represented as graphs.

In both machine learning and information theory literatures, there has been some work on learned coding. From a machine learning perspective, the paper [4] stated the problem precisely and developed and evaluated some algorithms. A few follow up papers, e.g., [5], [6], [7], [8], [9], [10] have introduced new machine learning algorithms. For lossy coding, in particular of images and video, there has been much more activity recently, initiated by the paper [11] from Google, see for example [12], [13], [14]. Our aim is to find theoretical bounds for how well it is possible to learn coding. In this paper we will limit ourselves to lossless coding.

From an information theory perspective, Hershkovits and Ziv [15] considered learned coding in terms of learning a database of sequences. The results in [15] are quite pessimistic. Basically they state that to code a sequence of length \( l \) so as to approach the entropy rate \( \mathcal{H} \), a length \( 2^{\mathcal{H}l} \) training sequence is needed – so that one observes most of the typical sequences. This means that essentially learned coding is infeasible, as the amount of training needed is exponential in the sequence length! Yet, machine learning has shown itself to work very well in other contexts with large, but not extreme training sets. We will therefore consider the problem from a different perspective.

Our perspective on learning coding is to compare with universal source coders with redundancy as measure. The redundancy of a coder is is the difference between the entropy of a source and the average length achieved by the coder. Suppose that the sources are (or assumed to be) in some probability class \( \Lambda \) characterized by a parameter vector \( \theta \). For a universal source coder with length function \( L \), the redundancy to encode a sequence of length \( l \) is defined by [16]

\[
R_c(L, \theta) = \frac{1}{l} E_\theta [L(X^l)] - H_\theta(X)
\]

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Since $\theta$ is unknown, even in terms of probability law, usually the minimax redundancy is considered \cite{16}
\[ R_*^+ = \min_L \sup_{\theta} R_l(L, \theta) \]

A good coder is one that achieves this minimum.

This setup can be generalized to learning. We are given a training sequence $x^m$; based on the training we develop coders $C(x^l; x^m)$ with length function $L(x^l; x^m)$. The codelength is $\frac{1}{n}E_\theta[L(x^l; x^m)|x^m]$ (the expectation here is only over $x^l$), and the redundancy is
\[ R_l(L, x^m, \theta) = \frac{1}{l}E_\theta[L(x^l; x^m)|x^m] - H_\theta(X) \] \hspace{1cm} (1)

The redundancy depends on the training sequence $x^m$. One way to remove this dependency is to average also over $x^m$,
\[ R_l(L, m, \theta) = \frac{1}{l}E_\theta[L(x^l; x^m)] - H_\theta(X) \] \hspace{1cm} (2)
\[ R_*^+(m) = \min_L \sup_{\theta} R_l(L, m, \theta) \] \hspace{1cm} (3)

The idea of learning to code is to obtain information about the distribution of the source from the training $x^m$ and then apply this to code the test sequence $x^l$. From a theoretical point of view of simply minimizing (3), one could say that of course the coder can continue to learn about the source from the test sequence. However, machine learning algorithms usually have a distinct learning phase, and once the algorithm is trained, it is not updated with test samples. We will therefore also consider this setup here, and we call such a learned coder a frozen coder. For the coders we consider this is easy to specify. From the training sequence $x^m$ the coder estimates a distribution $\hat{P}(\cdot)$ and this is then applied to test sequences, without updating, through a Shannon/algebraic coder resulting in $L(x^l) = -\log(\hat{P}(x^l))$ (ignoring a possible $+1$).

The question we consider now is: how many training samples do we need in order to beat a universal source coder, i.e., how large should $m$ be so that
\[ R_*^+(m) \leq R_*^+ \] \hspace{1cm} (4)

One might of course want better performance than a universal coder. But at least one would want the learned coder to do as well as a universal coder, so (4) gives a baseline on performance.

Learning to code has similarities with universal prediction \cite{17}. The paper \cite{18} developed bounds for universal prediction for IID (independent identically distributed) sources, and \cite{19}, \cite{20} for Markov sources. In fact, the paper \cite{18} exactly considers (3), and proves
\[ \frac{1}{2m \ln 2} + o\left(\frac{1}{m}\right) \leq R_*^+(m) \leq \frac{\alpha_0}{m \ln 2} + o\left(\frac{1}{m}\right) \] \hspace{1cm} (5)
\[ \alpha_0 \approx 0.50922 \] \hspace{1cm} (6)

The result was improved in \cite{21} to show that
\[ R_*^+(m) = \frac{1}{2m \ln 2} + o\left(\frac{1}{m}\right) \] \hspace{1cm} (7)

On the other hand, we also have good expressions for $R_*^+$ \cite{16}, which can be expressed as $R_*^+ = \frac{\log l}{2l} + o\left(\frac{1}{l}\right)$. Thus, ignoring $o$-terms, (4) becomes
\[ m \geq \frac{l}{\ln 2 \log l} \] \hspace{1cm} (8)

The conclusion is that it is very easy to beat a universal coder. For $l$ moderately large $\frac{l}{\ln 2 \log l} < l$, so we need fewer training samples than the length of the sequences we want to encode.
We now return to (2). Averaging over the training \( x^m \) might be reasonable for universal prediction. But in learning one usually learns once and applies many times. The average code length over test sequences in (1) is therefore reasonable, but the averaging over the training less so. As an alternative one could consider the worst case over \( x^m \), but one can always find totally non-informative training sequences (e.g., for the IID case the sequence of all zeros). Instead one could require that the training is good for most training sequences, or, put another way, that the probability of a bad training sequence is low. So, we consider the criterion

\[
E(m,a) = \sup_{\theta} P (R_{\ell}(L, x^m, \theta) > a)
\]  

(9)

For some given \( a \) and small \( P_e \) the goal is then to ensure

\[
E(m,a) \leq P_e
\]

Again, we can consider the bottom line of beating the universal coder, in which case \( a = \frac{\log l}{2l} \) for the IID case.

In this paper we consider the measure (9) for the IID binary case, and we then generalize to binary Markov chains for both the average measure (3) and the error measure (9).

II. IID Case

We consider the IID binary case characterized by the parameter \( \theta = p \), where \( p = P(X = 1) \) and \( q = 1 - p \). Learning an estimator boils down to finding an estimator \( \hat{p} \). It is then well known [3] that the redundancy of a coder defined by \( \hat{p} \) is \( R_{\ell}(L, x^m, \theta) = D(p \| \hat{p}) \) (except for some small constant), and therefore

\[
E(m,a) = \sup_p P (D(p \| \hat{p}) \geq a)
\]

Consider first the maximum likelihood estimator (MLE), \( \hat{p} = \frac{k}{m} \), where \( k \) is the number of ones in the training sequence \( x^m \). If \( k = 0 \), \( D(p \| \hat{p}) = \infty \), and at the same time \( \lim_{p \to 0} P(k = 0) = \lim_{p \to 0} (1 - p)^m = 1 \); therefore

**Proposition 1.** For the MLE, \( E(m,a) = 1 \) for all \( a > 0 \)

In light of Proposition [1] we consider other estimators \( \hat{p} \). We assume that \( \hat{p} = f(\hat{p}) \), where

\[
\hat{p} = \frac{k}{m}
\]

is the minimal sufficient statistic; the function \( f \) can depend on \( m \). For convenience, we assume \( f \) is invertible. Let

\[
P(p,a) = P (D(p \| \hat{p}) > a)
\]

for fixed \( p \leq \frac{1}{2} \). The equation \( D(p \| \hat{p}) = a \) has two solutions \( \hat{p}_{\pm} \) so that

\[
P(p,a) = P (\hat{p} < f^{-1}(\hat{p}_{-})) + P (\hat{p} > f^{-1}(\hat{p}_{+}))
\]

the sum of the lower and upper tail probabilities.

We consider what can be named the moderate deviations regime. We fix \( P_e \) independent of \( m \) and require \( E(m,a) \leq P_e \) and desire to find the smallest \( a(m, P_e) \) that satisfies this inequality. We solve the problem asymptotically as \( m \to \infty \); necessarily \( a(m, P_e) \to 0 \), and we want to find how it converges to zero. This essentially gives the redundancy as a function of \( m \). We can use this to determine how many training samples we need to beat universal source coding: solving \( a(m, P_e) < \frac{1}{2\log l} \).
Let $0 \leq \lambda \leq 1$ and put
\[
\hat{p}_-(p, m, \lambda P_e) = \inf \{ \hat{p} : P(\hat{p} < f^{-1}(\hat{p})) \leq \lambda P_e \}
\]
\[
\hat{p}_+(p, m, (1 - \lambda) P_e) = \sup \{ \hat{p} : P(\hat{p} > f^{-1}(\hat{p})) \leq (1 - \lambda) P_e \}
\]
Then we can write
\[
a(m, P_e) = \min_{\lambda} \sup_{p} \max \{ D(p\|\hat{p}_-(p, m, \lambda P_e)), D(p\|\hat{p}_+(p, m, (1 - \lambda) P_e)) \}
\tag{10}
\]
For achievability, we consider estimators of the well-known form \cite{3, 22, 18}
\[
\hat{p} = \frac{k + \beta m}{m + 2\beta m} = \frac{\hat{p} + \beta}{1 + 2\beta}
\tag{11}
\]
where, as we will see, for moderate deviations we can put $\beta = \frac{\alpha}{m}$, so that\footnote{The exact result \cite{7} was obtained by using a modified additive estimator, but we will limit the consideration here to the plain additive estimator.}
\[
\hat{p} = \frac{k + \frac{\alpha}{m}}{m + 2\frac{\alpha}{m}}
\tag{12}
\]
The main result is

\textbf{Theorem 1.} For estimators that are functions of the sufficient statistic and $P_e$ sufficiently small,
\[
a(m, P_e) \geq \frac{Q^{-1}(P_e/2)^2}{2m \ln 2} + o \left( \frac{1}{m} \right)
\tag{13}
\]
The estimator \cite{12} has an optimum value of $\alpha$ that satisfies
\[
\frac{1}{6} Q^{-1}(P_e/2)^2 - 1 \leq \alpha \leq \frac{1}{6} Q^{-1}(P_e/2)^2 + 1
\tag{14}
\]
which gives an achievable $a(m, P_e)$;
\[
a(m, P_e) = b(P_e) \frac{Q^{-1}(P_e/2)^2}{2m \ln 2} + o \left( \frac{1}{m} \right)
\tag{15}
\]
where
\[
\lim_{P_e \to 0} b(P_e) = 1
\]
\textit{Proof.} We will first argue that we can focus on convergent sequences in the proof technique. We want to find the limit $\lim_{m \to \infty} ma(m, P_e)$ (implicitly a $\lim \sup$). Let $p_{\max}(m)$ be a value of $p$ where $a(m, P_e)$ is achieved – if there are multiple, we choose one at random. Consider the sequence $mp_{\max}(m)$; it has at least one accumulation point when $\infty$ is included. Again we choose one a random, and a subsequence $m'p_{\max}(m')$ that converges towards the accumulation point. It is clear that $\lim_{m' \to \infty} m'a(m', P_e) = \lim_{m \to \infty} ma(m, P_e)$. We can therefore equivalently find the maximum of $ma(m, P_e)$ along convergent sequences $mp(m)$. We can divided such sequences into three regimes:
- **CLT regime**: $\lim_{m \to \infty} mp(m) = \infty$. In this regime the central limit theorem (CLT) can be applied.
- **Poisson regime**: $0 < \lim_{m \to \infty} mp(m) < \infty$. In this regime a Poisson approximation can be used.
- **Sub-Poisson regime**: $\lim_{m \to \infty} mp(m) = 0$.
We consider the limit of $ma(m, P_e)$ in each of these regimes, and maximizes over these limits. In the following we will drop the explicit dependency $p(m)$ and just write $p$. 
CLT Regime: We can then use the central limit theorem, here for the upper tail,
\[
P(\hat{p} > f^{-1}(\hat{p}_+)) = P(\hat{p} - p > f^{-1}(\hat{p}_+) - p)
\]
\[
= P \left( \frac{\sqrt{m}}{\sqrt{pq}} (\hat{p} - p) > \frac{\sqrt{m}}{\sqrt{pq}} (f^{-1}(\hat{p}_+) - p) \right)
\]
\[
\rightarrow Q \left( \lim_{m \to \infty} \frac{\sqrt{m}}{\sqrt{pq}} (f^{-1}(\hat{p}_+) - p) \right) \quad \text{as } m \to \infty
\]
(16)
(with \(Q(x) = 1 - \Phi(x), \Phi\) being the Gaussian CDF) as Berry-Esseen [23] gives
\[
\left| P(\hat{p} < f^{-1}(\hat{p}_+)) - \Phi \left( \frac{\sqrt{m}}{\sqrt{pq}} (f^{-1}(\hat{p}_+) - p) \right) \right| \leq 0.4274 \frac{p^2 + q^2}{\sqrt{mpq}}
\]
(17)
and the right hand side converges to zero by assumption. We require
\[
P(\hat{p} > f^{-1}(\hat{p}_+)) = Q \left( \frac{\sqrt{m}}{\sqrt{pq}} (f^{-1}(\hat{p}_+) - p) \right) + \epsilon(m) \leq (1 - \lambda)P_e
\]
where \(\lim_{m \to \infty} \epsilon(m) = 0\) from (17). We can include the gap in the inequality in \(\epsilon(m)\), so
\[
Q \left( \frac{\sqrt{m}}{\sqrt{pq}} (f^{-1}(\hat{p}_+) - p) \right) = (1 - \lambda)P_e + \epsilon(m)
\]
and thus
\[
\hat{p}_+ = f \left( \frac{\sqrt{pq}}{\sqrt{m}} Q^{-1}((1 - \lambda)P_e + \epsilon(m)) + p \right)
\]
In the following we will omit the \(\epsilon(m)\) as it does not affect the results.
We will first consider a converse in the CLT regime, more specifically for \(p\) constant rather than a function of \(m\). This is clearly also a converse for all regimes. We use Pinsker’s inequality for relative entropy [24],
\[
D(p\|\hat{p}_+) \geq \frac{2}{\ln 2} (p - \hat{p}_+)^2
\]
(18)
in (10)
\[
a(m, P_e) \geq \frac{2}{\ln 2} \min \min \sup \max \left\{ \left( f \left( \frac{\sqrt{pq}}{\sqrt{m}} Q^{-1}((1 - \lambda)P_e) + p \right) - p \right)^2, \right.
\]
\[
\left. \left( f \left( -\frac{\sqrt{pq}}{\sqrt{m}} Q^{-1}(\lambda P_e) + p \right) - p \right)^2 \right\}
\]
(19)
Let \(f(x) = x + g_m(x)\), where we have made explicit that \(f\) can depend on \(m\). We can then write this as
\[
a(m, P_e) \geq \frac{2}{m \ln 2} \min \min \sup \max \left\{ \left( \sqrt{pq}Q^{-1}((1 - \lambda)P_e) + \sqrt{m}g_m \left( \frac{\sqrt{pq}}{\sqrt{m}} Q^{-1}((1 - \lambda)P_e) + p \right) \right)^2, \right.
\]
\[
\left. \left( -\sqrt{pq}Q^{-1}(\lambda P_e) + \sqrt{m}g_m \left( -\frac{\sqrt{pq}}{\sqrt{m}} Q^{-1}(\lambda P_e) + p \right) \right)^2 \right\}
\]
(20)
We will argue that \(g_m = 0\) and \(\lambda = \frac{1}{2}\) is optimum, or more precisely that \(\lim_{m \to \infty} \sqrt{m}g_m = 0\). Suppose that for some \(p\), \(\lim_{m \to \infty} \sqrt{m}g_m \left( \frac{\sqrt{pq}}{\sqrt{m}} Q^{-1}((1 - \lambda)P_e) + p \right) = b\), so that
\[
\lim_{m \to \infty} \left( \sqrt{pq}Q^{-1}((1 - \lambda)P_e) + \sqrt{m}g_m \left( \frac{\sqrt{pq}}{\sqrt{m}} Q^{-1}((1 - \lambda)P_e) + p \right) \right)^2
\]
\[
= \left( \sqrt{pq}Q^{-1}((1 - \lambda)P_e) + b \right)^2
\]
Let $p_m$ be the solution to
\[-\frac{\sqrt{pq}}{\sqrt{m}}Q^{-1}(\lambda P_e) + p_m = \frac{\sqrt{pq}}{\sqrt{m}}Q^{-1}((1 - \lambda)P_e) + p.\]

Then
\[
\lim_{m \to \infty} \left( -\sqrt{pq}mQ^{-1}(\lambda P_e) + \sqrt{mqm} \left( \frac{\sqrt{pq}}{\sqrt{m}}Q^{-1}((1 - \lambda)P_e) + p_m \right) \right)^2
= \left( -\frac{\sqrt{pq}Q^{-1}(\lambda P_e) + b}{2} \right)^2
\]

Thus the maximum in (20) as $m \to \infty$ becomes
\[
\max \left\{ \left( \frac{\sqrt{pq}}{\sqrt{m}}Q^{-1}((1 - \lambda)P_e) + b \right)^2, \left( -\frac{\sqrt{pq}Q^{-1}(\lambda P_e) + b}{2} \right)^2 \right\}
\]
(21)

Since there is a minimization over $f$ and $\lambda$, we can choose $\lambda$ and $b$. It is now easily seen that (21)
is minimized for $\lambda = \frac{1}{2}$ and $b = 0$ as follows. We can assume that $P_e < \frac{1}{2}$ so that $Q^{-1}(P_e) > 0$.For $b = 0, \lambda = \frac{1}{2}$, the two parts of the max are equal. If we make $b > 0$ we must decrease $\lambda$ below $\frac{1}{2}$ to get $\left( \frac{\sqrt{pq}Q^{-1}((1 - \lambda)P_e) + b}{2} \right)^2 < \left( -\frac{\sqrt{pq}Q^{-1}(\lambda P_e) + b}{2} \right)^2$; but for such $\lambda$, $\left( -\frac{\sqrt{pq}Q^{-1}(\lambda P_e) + b}{2} \right) > \left( \frac{\sqrt{pq}Q^{-1}(\lambda P_e) + b}{2} \right)^2$ due to the convexity of $Q^{-1}(x)$ for $x < \frac{1}{2}$.

Thus, in (19) the minimum is achieved for $f$ the identity and $\lambda = \frac{1}{2}$, while the maximum over $p$ is achieved for $p = q = \frac{1}{2}$. This gives (15) as a lower bound.

For achievability in the CLT regime we explicitly have
\[
\hat{p}_+ = \frac{1}{1 + 2\frac{\alpha}{m}} \left( \frac{\sqrt{pq}}{\sqrt{m}}Q^{-1}(P_e/2) + p + \frac{\alpha}{m} \right)
\]
\[
\hat{p}_- = \frac{1}{1 + 2\frac{\alpha}{m}} \left( -\frac{\sqrt{pq}}{\sqrt{m}}Q^{-1}(P_e/2) + p + \frac{\alpha}{m} \right)
\]
(22)

Notice that in general $D(p_1||p_2)$ is an increasing function of the distance $|p_1 - p_2|$, and therefore $D(p||\hat{p}_\pm)$ for fixed $m$ are increasing functions of $p$ for $p \in (0, \frac{1}{2})$ as the distance $|p - \hat{p}_\pm|$ is given by $\frac{\sqrt{pq}}{\sqrt{m}}Q^{-1}(P_e/2) \pm \frac{\alpha}{m}$. We can therefore obtain the worst case achievable $a(m, P_e)$ by series expansion of $D(p||\hat{p}_\pm)$ for $p = \frac{1}{2}$,

\[
D(p||\hat{p}_\pm) = \frac{(p - \hat{p}_\pm)^2}{pq \ln 4} + o((p - \hat{p}_\pm)^2)
\]

which when inserting (22) achieves (15).

**Sub-Poisson regime:** In this regime $p = o(\frac{1}{m})$. Since $\hat{p}_- < p$, also $\hat{p}_- = o(\frac{1}{m})$. The lower tail probability is

\[
P \left( \hat{p} < f^{-1}(\hat{p}_-) \right) = P \left( \hat{p} < \hat{p}_- \left( 1 + 2\frac{\alpha}{m} \right) - \frac{\alpha}{m} \right)
= P \left( k < m\hat{p}_- \left( 1 + 2\frac{\alpha}{m} \right) - \alpha \right)
\]

For $m$ sufficiently large, the right hand side becomes negative, and therefore the probability zero. We therefore only have the constraint $P(\hat{p} > f^{-1}(\hat{p}_+)) \leq P_e$. Write

\[
P \left( \hat{p} > f^{-1}(\hat{p}_+) \right) = P \left( \hat{p} > \hat{p}_+ \left( 1 + 2\frac{\alpha}{m} \right) - \frac{\alpha}{m} \right)
= P \left( k > m\hat{p}_+ \left( 1 + 2\frac{\alpha}{m} \right) - \alpha \right)
\]

If $m\hat{p}_+ \to 0$ the probability converges to one. So, let $\hat{p}_+ = \frac{\alpha + \delta}{m}$ with $\delta > 0$ arbitrarily small, so that

\[
P \left( \hat{p} > f^{-1}(\hat{p}_+) \right) = P \left( k > (\alpha + \delta) \left( 1 + 2\frac{\alpha}{m} \right) - \alpha \right)
\]
(23)
As $P(k = 0) = (1 - p)^m = (1 - o(\frac{1}{m}))^m \to 1$ as $m \to \infty$ the probability converges to zero, i.e., is less than $P_e$ for $m$ sufficiently large so that the constraint is satisfied. We bound relative entropy by $\chi^2$-distance, see e.g. [24],

$$D(p\|\hat{p}_+) \leq \frac{(p - \hat{p}_+)^2}{\hat{p}(1 - \hat{p}_+) \ln 2}$$
$$\leq \frac{(1 - \frac{p}{\hat{p}_+})^2}{\hat{p}_+(1 - \hat{p}_+) \ln 2}$$
$$= \frac{\alpha + \delta}{m \ln 2} + o\left(\frac{1}{m}\right)$$

(24)

because $\frac{p}{\hat{p}_+} \to 0$.

**Poisson regime:** Let $p = \frac{\gamma}{m}$. We also set $\kappa_{\pm} = m\hat{p}_{\pm}$. Then

$$D\left(\frac{\gamma}{m} \biggm| \kappa_{\pm} \right) = \frac{\kappa_{\pm} - \gamma + \gamma \ln \gamma - \gamma \ln \kappa_{\pm}}{m \ln 2} + o\left(\frac{1}{m}\right)$$

(25)

We define

$$d(x, y) = y - x + x \ln \frac{x}{y}$$

Now

$$P\left(\hat{p} \leq f^{-1}(\hat{p}_-)ight) = P\left(\hat{p} \leq \hat{p}_-(1 + 2\beta) - \beta\right)$$
$$= P\left(k \leq \kappa_- \left(1 + \frac{2\alpha}{m}\right) - \alpha\right)$$
$$\to P_\gamma(\kappa_- - \alpha)$$

where $P_\gamma$ is the Poisson CDF. Similarly

$$P\left(\hat{p} > f^{-1}(\hat{p}_-)ight) \to 1 - P_\gamma(\kappa_+ - \alpha)$$

A reminder about the meaning of $\kappa_{\pm}$: for every $\gamma$, $\kappa_- = \sup \{\kappa : P_\gamma(\kappa - \alpha) \leq P_e/2\}$, and $\kappa_+ = \inf \{\kappa : P_\gamma(\kappa - \alpha) \geq 1\}$.

Figure 1 illustrates the proof.

![Figure 1](image-url)

Figure 1. Plot of $d(\tilde{\gamma}, \tilde{\kappa}_-), d(\tilde{\gamma}, \tilde{\kappa}_+)$ for $P_e = 10^{-6}$ for $\alpha = \frac{1}{6} Q^{-1}(P_e/2)^2 - 1$. The solid curves are for the exact values of $\kappa_{\pm}$, while the dashed curves are the bounds. The solid curves are sawtooth like, but this cannot be seen at the scale of the figures. The bounds are for the peaks of the solid curves.
We will first analyze the lower tail probability corresponding to $\kappa_-$. Let $\gamma_k, k = 0, 1, \ldots$ be the sequence of solutions $\mathbb{P}_{\gamma_k}(k) = \frac{P_e}{2} -$ these correspond to the peaks in the solid blue curve in Fig. 1. Notice that if $\gamma_{k-1} < \gamma \leq \gamma_k$, $|\gamma - k| \leq |\gamma_k - k|$, and this is also true for other distance measures. Now, according to (25),

$$
P_e = \mathbb{P}_{\gamma_k}(k) < \Phi \left( \text{sign}(k + 1 - \gamma_k) \sqrt{2d(k + 1, \gamma_k)} \right)
$$

so that

$$
\frac{1}{2} \Phi^{-1}(P_e/2)^2 > d(k + 1, \gamma_k)
$$

(since $k + 1 < \gamma_k$). As $\kappa_- = k + \alpha$, we therefore have

$$
d(\kappa_- - \alpha + 1, \gamma) < \frac{1}{2} \Phi^{-1}(P_e/2)^2 = \frac{1}{2} Q^{-1}(P_e/2)^2
$$

$$
\gamma - (\kappa_- - \alpha + 1) + (\kappa_- - \alpha) \ln \frac{\kappa_- - \alpha + 1}{\gamma} < \frac{1}{2} Q^{-1}(P_e/2)^2
$$

by normalizing by $Q^{-1}(P_e/2)^2$ we get

$$
d(\tilde{\kappa}_- - \tilde{\alpha}_-, \tilde{\gamma}) = \tilde{\gamma} - (\tilde{\kappa}_- - \tilde{\alpha}_-) + (\tilde{\kappa}_- - \tilde{\alpha}_-) \ln \frac{\tilde{\kappa}_- - \tilde{\alpha}_-}{\tilde{\gamma}} < \frac{1}{2}
$$

(26)

where specifically $\tilde{\alpha}_- = \frac{\alpha - 1}{Q^{-1}(P_e/2)^2}$. From (25) it can be seen that $a(m, P_e)$ is determined by the swapped relative entropy, $d(\tilde{\gamma}, \tilde{\kappa}_-)$. Solving (26) with equality we get

$$
\tilde{\kappa}_- - \tilde{\alpha}_- = r_- (\tilde{\gamma}) \tilde{\gamma} = \frac{\frac{1}{2\tilde{\gamma}} - 1}{W_{-1} \left( \frac{1}{e} \left( \frac{1}{2\tilde{\gamma}} - 1 \right) \right)} \tilde{\gamma}
$$

(27)

where $W_{-1}$ is the Lambert $W$-function of order $-1$.

For the upper tail probability, we instead define $\lambda_k, k = 0, 1, \ldots$ as the sequence of solutions $\mathbb{P}_{\lambda_k}(k) = 1 - \frac{P_e}{2}$. We use the lower bound from (25),

$$
1 - \frac{P_e}{2} = \mathbb{P}_{\gamma_k}(k) > \Phi \left( \text{sign}(k + 1 - \gamma_k) \sqrt{2d(k, \gamma_k)} \right)
$$

$$
d(k, \gamma_k) < \frac{1}{2} \Phi^{-1}(1 - P_e/2)^2 = \frac{1}{2} Q^{-1}(P_e/2)^2
$$

We then have

$$
\tilde{\gamma} - (\tilde{\kappa}_+ - \tilde{\alpha}_+) + (\tilde{\kappa}_+ - \tilde{\alpha}_+) \ln \frac{\tilde{\kappa}_+ - \tilde{\alpha}_+}{\tilde{\gamma}} < \frac{1}{2}
$$

(28)

where now $\tilde{\alpha}_+ = \frac{\alpha + 1}{Q^{-1}(P_e/2)^2}$. The solution of (28) with equality is

$$
\tilde{\kappa}_+ - \tilde{\alpha}_+ = r_+ (\tilde{\gamma}) \tilde{\gamma} = \frac{\frac{1}{2\tilde{\gamma}} - 1}{W_0 \left( \frac{1}{e} \left( \frac{1}{2\tilde{\gamma}} - 1 \right) \right)} \tilde{\gamma}
$$

(29)

The problem is now reduced to finding

$$
\sup_{\gamma > 0} \max \left\{ d(\tilde{\gamma}, \tilde{\kappa}_-), d(\tilde{\gamma}, \tilde{\kappa}_+) \right\} \triangleq \frac{1}{2} b(P_e)
$$

(30)

$$
d(\tilde{\kappa}_- - \tilde{\alpha}_-, \tilde{\gamma}) = \frac{1}{2}
$$

$$
d(\tilde{\kappa}_+ - \tilde{\alpha}_+, \tilde{\gamma}) = \frac{1}{2}
$$

While (25) states the bounds for $k = 1, 2, \ldots$, it is easy to see that the bounds are also valid for $k = 0$, and the upper bound is also valid or non-integer values of $k$. 
We notice that $d(\bar{\gamma}, \bar{\kappa}_-)$ is decreasing with $\alpha$ while $d(\bar{\gamma}, \bar{\kappa}_+)$ is increasing. We will first show that if $\bar{\alpha}_+ \leq \bar{\alpha}_+^*$ for some $\bar{\alpha}_+^*$, then $\sup_{\bar{\gamma}} d(\bar{\gamma}, \bar{\kappa}_+) \leq \frac{1}{2}$.

By inserting (29) in $d(\bar{\gamma}, \bar{\kappa}_+)$ we find that (Mathematica)

$$
\lim_{\bar{\gamma} \to \infty} \bar{\kappa}_+ - \bar{\gamma} + \bar{\gamma} \ln \frac{\bar{\gamma}}{\bar{\kappa}_+} = \frac{1}{2}
$$

(31)

We will now prove that if $\bar{\alpha}_+ \leq \bar{\alpha}_+^*$ and $d(\bar{\gamma}, \bar{\kappa}_+) > \frac{1}{2}$, then $d(\bar{\gamma}, \bar{\kappa}_+)$ is increasing in $\bar{\gamma}$, which would then contradict the limit (31).

Let $\bar{\kappa}_+ = f(\bar{\gamma})$ be the solution (29). The derivative of $d(\bar{\gamma}, \bar{\kappa}_+)$ is

$$
f'(\bar{\gamma}) + \ln \frac{\bar{\gamma}}{f(\bar{\gamma})} + \bar{\gamma} \frac{f'(\bar{\gamma})}{f(\bar{\gamma})} \geq 0
$$

where we want to show the inequality. The implicit function theorem gives,

$$
f'(\bar{\gamma}) = \frac{\frac{\bar{\gamma}}{\bar{\kappa}_+ - \bar{\alpha}_+} - 1}{\ln \frac{\bar{\kappa}_+ - \bar{\alpha}_+}{\bar{\gamma}}}
$$

Thus, to show that $d(\bar{\gamma}, \bar{\kappa}_+)$ is increasing we have to show

$$
\bar{\kappa}_+ \left( \bar{\gamma} \ln \left( \frac{\bar{\gamma}}{\bar{\kappa}_+} \right) \ln \left( \frac{\bar{\kappa}_+ - \bar{\alpha}_+}{\bar{\gamma}} \right) + (\bar{\kappa}_+ - \bar{\alpha}_+) - \bar{\gamma} \right) + \bar{\gamma}(\bar{\gamma} - (\bar{\kappa}_+ - \bar{\alpha}_+)) \\
\bar{\gamma} \bar{\kappa}_+ \ln \left( \frac{\bar{\kappa}_+ - \bar{\alpha}_+}{\bar{\gamma}} \right) \geq 0
$$

(32)

which reduces to

$$
\bar{\kappa}_+ \left( \bar{\gamma} \ln \left( \frac{\bar{\gamma}}{\bar{\kappa}_+} \right) \ln \left( \frac{\bar{\kappa}_+ - \bar{\alpha}_+}{\bar{\gamma}} \right) \right) \geq (\bar{\kappa}_+ - \bar{\gamma})(\bar{\gamma} - (\bar{\kappa}_+ - \bar{\alpha}_+))
$$

As stated above, we assume that $\bar{\kappa}_+ - \bar{\gamma} + \bar{\gamma} \ln \frac{\bar{\gamma}}{\bar{\kappa}_+} \geq \frac{1}{2}$, or $\bar{\gamma} \ln \frac{\bar{\gamma}}{\bar{\kappa}_+} \geq \frac{1}{2} - (\bar{\kappa}_+ - \bar{\gamma})$. Inserting, we have to prove

$$
\bar{\kappa}_+ \left( \left( \frac{1}{2} - (\bar{\kappa}_+ - \bar{\gamma}) \right) \ln \left( \frac{\bar{\kappa}_+ - \bar{\alpha}_+}{\bar{\gamma}} \right) \right) \geq (\bar{\kappa}_+ - \bar{\gamma})(\bar{\gamma} - (\bar{\kappa}_+ - \bar{\alpha}_+))
$$

From (28) with equality we have

$$
(\bar{\kappa}_+ - \bar{\alpha}_+) \ln \left( \frac{\bar{\kappa}_+ - \bar{\alpha}_+}{\bar{\gamma}} \right) = (\bar{\kappa}_+ - \bar{\alpha}_+) - \bar{\gamma} + \frac{1}{2}
$$

or

$$
\bar{\kappa}_+ \ln \left( \frac{\bar{\kappa}_+ - \bar{\alpha}_+}{\bar{\gamma}} \right) = (\bar{\kappa}_+ - \bar{\alpha}_+) - \bar{\gamma} + \frac{1}{2} + \bar{\alpha}_+ \ln \left( \frac{\bar{\kappa}_+ - \bar{\alpha}_+}{\bar{\gamma}} \right)
$$

(33)

then we have the following sequence of inequalities

$$
\left( \left( \frac{1}{2} - (\bar{\kappa}_+ - \bar{\gamma}) \right) \left( (\bar{\kappa}_+ - \bar{\alpha}_+) - \gamma + \frac{1}{2} + \bar{\alpha}_+ \ln \left( \frac{\bar{\kappa}_+ - \bar{\alpha}_+}{\bar{\gamma}} \right) \right) \right) \geq (\bar{\kappa}_+ - \bar{\gamma})(\bar{\gamma} - (\bar{\kappa}_+ - \bar{\alpha}_+))
$$

$$
\left( \frac{1}{2} - (\bar{\kappa}_+ - \bar{\gamma}) \right) \left( \frac{1}{2} + \bar{\alpha}_+ \ln \left( \frac{\bar{\kappa}_+ - \bar{\alpha}_+}{\bar{\gamma}} \right) \right) \geq \frac{1}{2}(\bar{\gamma} - (\bar{\kappa}_+ - \bar{\alpha}_+))
$$

$$
\left( \bar{\gamma} - (\bar{\kappa}_+ - \frac{1}{2}) \right) \left( \frac{1}{2} + \bar{\alpha}_+ \ln \left( \frac{\bar{\kappa}_+ - \bar{\alpha}_+}{\bar{\gamma}} \right) \right) \geq \frac{1}{2}(\bar{\gamma} - (\bar{\kappa}_+ - \bar{\alpha}_+))
$$

$$
\left( \bar{\kappa}_+ - \frac{1}{2} - \bar{\gamma} \right) \left( \frac{1}{2} + \bar{\alpha}_+ \ln \left( \frac{\bar{\kappa}_+ - \bar{\alpha}_+}{\bar{\gamma}} \right) \right) \leq \frac{1}{2}((\bar{\kappa}_+ - \bar{\alpha}_+) - \bar{\gamma})
$$

$$
\bar{\alpha}_+ \left( \left( r_+(\bar{\gamma}) - 1 \right) \bar{\gamma} + \bar{\alpha}_+ - \frac{1}{2} \right) \ln \left( r_+(\bar{\gamma}) \right) \leq \frac{1}{2} \left( \frac{1}{2} - \bar{\alpha}_+ \right)
$$

(34)
This is a second order inequality in $\tilde{\alpha}_+$, which can be solved to give $\tilde{\alpha}_+ \leq f(\tilde{\gamma})$, where $f(\tilde{\gamma})$ is a rather large expression that we will not write down here. The function $f(\tilde{\gamma})$ is decreasing, and it can be shown (Mathematica) that $\lim_{\tilde{\gamma} \to \infty} f(\tilde{\gamma}) = \frac{1}{\gamma}^\gamma$.

We now argue by contradiction. Let $\tilde{\alpha}_+ \leq \frac{1}{6}$. If at some time $\tilde{k}_+ - \tilde{\gamma} + \tilde{\gamma} \ln \frac{\tilde{\gamma}}{\tilde{k}_+} > \frac{1}{2}$ then $\tilde{k}_+ - \tilde{\gamma} + \tilde{\gamma} \ln \frac{\tilde{\gamma}}{\tilde{k}_+}$ is increasing, thus it stays strictly above $\frac{1}{2}$. But then the limit (31) cannot be achieved. Thus we conclude that we must have $\tilde{k}_+ - \tilde{\gamma} + \tilde{\gamma} \ln \frac{\tilde{\gamma}}{\tilde{k}_+} \leq \frac{1}{2}$.

For the lower tail, the above argument can be repeated, where we now have $\tilde{\alpha}_- \geq f(\tilde{\gamma})$ with $f(\tilde{\gamma})$ the solution of (34) with $r_2(\tilde{\gamma})$ replaced with $r_+(\tilde{\gamma})$ given by (27). It turns out that in this case also $\lim_{\tilde{\gamma} \to \infty} f(\tilde{\gamma}) = \frac{1}{\gamma}^\gamma$.

Since $\tilde{\alpha}_- < \tilde{\alpha}_+$ we cannot have both $\tilde{\alpha}_- \geq \frac{1}{6}$ and $\tilde{\alpha}_+ \leq \frac{1}{6}$. However, we can choose $\alpha$ so that both $\lim_{P_\alpha \to 0} \tilde{\alpha}_+ = \lim_{P_\alpha \to 0} \tilde{\alpha}_+ = \frac{1}{6}$, and therefore in the limit both $\sup_{\gamma > 0} d(\tilde{\gamma}, \tilde{k}_+)$, $\sup_{\gamma > 0} d(\tilde{\gamma}, \tilde{k}_-) \leq \frac{1}{2}$. This shows that $b(P_\alpha)$ given by (30) converges to 1 as $m \to \infty$.

To summarize: in the CLT regime we get the achievable $\lim_{m \to \infty} ma(m, P_e) = \frac{Q^{-1}(P_e)}{2 \ln 2}$, in the Poisson regime $\lim_{m \to \infty} ma(m, P_e) = b(P_e) \frac{Q^{-1}(P_e)}{2 \ln 2}$ when $\alpha$ chosen as (14), and in the sub-Possion regime (24) $\lim_{m \to \infty} ma(m, P_e) = \frac{a + \delta}{\ln 2}$ with $\delta > 0$ arbitrarily small, which is smaller than $\frac{Q^{-1}(P_e)}{2 \ln 2}$ with this choice of $\alpha$. Thus, the Poisson regime gives the worst performance and results in (15).

The first thing to notice from this result is that as for average performance, the performance increases as $\frac{1}{m}$. Specifically, to beat universal coding of sequences of maximum length $l$ with probability $1 - P_e$ the number of training samples is approximately

$$m \geq \frac{Q^{-1}(P_e/2)^2}{2 \ln 2} \frac{l}{\log l}$$

Comparing this with (8) we can see that $m$ still increases as $\frac{l}{\log l}$, which is very moderate. However, the factor in front can be large. Additionally, the optimum value of $\alpha$ is different; for the average case $\alpha \approx \frac{1}{2}$ (6), while here $\alpha \approx \frac{1}{6} Q^{-1}(P_e/2)^2$, which can be considerably larger. The purpose of $\alpha$ is to avoid that rarely seen symbols require extremely long codewords. We can therefore interpret this so that to keep training error very small, protection against long codewords is of even higher importance then for average performance.

The other thing to remark is that the upper and lower bounds are only tight in the limit: they are separated by a factor $b(P_e)$. This factor is determined by how much the curves in Fig. 1 “bump” above the $\frac{1}{2} Q^{-1}(P_e/2)$ line. The figure shows a case where the upper tail probability stays completely below the line, so that $b(P_e)$ is completely determined by the bump of the lower tail probability. If one increases $\alpha$, the lower tail bump becomes smaller and the upper tail curve will develop a bump. Eventually at the upper range of (14) the lower tail probability will be completely below the line, and $b(P_e)$ will be determined completely by the bump on the upper tail probability. It is clear that if one wants an accurate value of $b(P_e)$ one can optimize over $\alpha$ in this range, and one can even use the exact probability rather than the bounds. But the numerical computation is not easy and might become unstable for small values of $P_e$.

Instead we suggest to calculate an upper bound on $b(P_e)$ by choosing $\alpha$ as the lower bound of (14) so that $b(P_e)$ is determined by the bump of the lower tail, which can be calculated by

$$b(P_e) \leq 2 \max_{\tilde{\gamma} > 0} \tilde{k}_- - \tilde{\gamma} + \tilde{\gamma} \ln \tilde{\gamma} - \tilde{\gamma} \ln \tilde{k}_-$$

where $\tilde{k}_-$ is given by (27), explicitly

$$\tilde{k}_- = \frac{\frac{1}{2\tilde{\gamma}} - 1}{W_1\left(\frac{1}{e}\left(\frac{1}{2\tilde{\gamma}} - 1\right)\right)} \tilde{\gamma} + \frac{1}{6} - \frac{2}{Q^{-1}(P_e/2)^2}$$

This maximization in (36) then easily can be done numerically. A plot of this upper bound on $b(P_e)$ can be seen in Fig. 2 below.
III. EXTENSION TO MARKOV CHAINS

We consider a binary Markov with states 0, 1. Let \( p_i = p(i|i) \) be the probability of staying in state \( i \) when the current state is \( i \). The stationary probability is

\[
\pi_i = \frac{p_i}{p_0 + p_1}
\]

Based on training, estimates \( \hat{p}_0 \) and \( \hat{p}_1 \) are generated. The redundancy for coding then is

\[
\pi_0 D(p_0 \| \hat{p}_0) + \pi_1 D(p_1 \| \hat{p}_1)
\]

We consider the two measures of performance

\[
R_i^+(m) = \sup_{p_0, \hat{p}_1} E \left[ \pi_0 D(p_0 \| \hat{p}_0) + \pi_1 D(p_1 \| \hat{p}_1) \right]
\]

\[
E(m, a) = \sup_{p_0, \hat{p}_1} P \left( \pi_0 D(p_0 \| \hat{p}_0) + \pi_1 D(p_1 \| \hat{p}_1) \geq a \right)
\]

As in the proof of Theorem [1], we consider convergent sequences \((p_0(m), p_1(m))\). From this we also have a limit \( \pi_i = \lim_{m \to \infty} \pi_i(m) \). If \( \pi_0 = 0 \), only the term corresponding to \( \pi_1 \) in (37) matters; it is therefore reduced to the iid case, which has better performance. We can therefore assume that \( \pi_i \neq 0 \).

In [19], [20] universal prediction (called estimation) for Markov chains was considered, as an extension of [18]. It was shown that the estimation error decreases as \( \frac{\log \log m}{m} \), which is an interesting contrast to (5). However, for learned coding the redundancy does not decrease at all with the length of the training sequence.

**Proposition 2.** Assume that the training data consists of a single sequence. Then

\[
R(m) \geq \frac{1}{2}
\]

\[
E(m, a) = 1 \quad \text{for} \quad a < \frac{1}{2}
\]

**Proof.** Let \( p_1 = p_0 \). The probability that a training sequence never changes state is then \((1 - p_0)^m\). Let us assume that the training sequence is in state 0, and that it uses this to generate a perfect estimate \( \hat{p}_0 = p_0 \). Since no example of state 1 is seen, the best minimax estimate of \( \hat{p}_1 \) is \( \hat{p}_1 = \frac{1}{2} \). Then

\[
E \left[ \pi_0 D(p_0 \| \hat{p}_0) + \pi_1 D(p_1 \| \hat{p}_1) \right] \geq (1 - p_0)^m \frac{1}{2} (1 - H(p_0)) \rightarrow \frac{1}{2} \quad \text{as} \quad p_0 \rightarrow 0
\]

Similarly

\[
P \left( \pi_0 D(p_0 \| \hat{p}_0) + \pi_1 D(p_1 \| \hat{p}_1) \geq \frac{1}{2} (1 - H(p_0)) \right) \geq (1 - p_0)^m
\]

The different behavior is easy to understand intuitively. If the Markov chain is slow mixing, the training sequence might see only one state. But the test sequence could be from the other state, about which nothing has been learned. On the other hand, in universal prediction, the goal is to predict the next sample after a training sequence. If the training sequence has seen only a single state, there is a good chance the following sample is also from that state, so prediction is not too bad. The point is that universal prediction and learned coding are not quite equivalent.

From the above it is clear that multiple training sequences are required for learning how to code. For achievability, we let the training data consist of \( n \) sequences of length \( l \). We assume that each sequence has an initial state according to the stationary distribution. Let \( \bar{m}_i \) be the number of visits to state \( i \); this is of course random, but converges towards \( \pi_i m \) by the law of large numbers. In order to handle this randomness in the estimators, we consider genie assisted estimators. For achievability we consider an
estimator that is inhibited by the genie as follows. The genie fixes \( m_i \) with \( m_1 + m_0 \leq m - n \) and inhibits the estimation as follows

- If there are more than \( m_i \) visits to state \( i \), it only uses the first \( m_i \) ones to estimate \( p_i \).
- If there is either less than \( m_0 \) visits to state \( 0 \) or less than \( m_1 \) visits to state \( 1 \), the genie generates more training data with the correct distribution until there is the correct number of visits; however, it also marks the sequence as invalid.

In either case we use the estimator (12) to estimate

\[
\hat{p}_i = \frac{k_{ii} + \alpha}{m_i + 2\alpha}
\]

where \( k_{ii} \) is the number of times the sequence stays in state \( i \) out of the \( m_i \) visits to state \( i \). This estimator is of course not realizable; a realizable estimator is one that uses (39) based on the actual number of visits \( \hat{m}_i \). But the way we have constructed the genie-inhibited estimator means that the realizable estimator has at least as good performance.

For the converse, we assume that the genie makes training data that has exactly \( m_i \) visits to state \( i \) with \( m_1 + m_0 = m \). We optimize the estimator over \( m_1, m_0 \); thus there is no assumption that sequences start according to the stationary distribution.

Denote by \( E_2 \) the event that the genie marks a sequence as invalid. We now bound \( P(E_2) \). Let

\[
m_i = (\pi_i - \epsilon)(m - n)
\]

and let \( \hat{m}_i \) be the actual number of visits to state \( i \). Then

\[
P(E_2) = P(\hat{m}_0 < m_0 \lor \hat{m}_1 < m_1)
\]

We then have

**Lemma 2.** With \( m_i \) given by (40) and \( P(E_2) \) by (41) we can bound

\[
P(E_2) \leq 2 \exp(-2n\epsilon^2)
\]

for all \( p_0, p_1 \).

**Proof.** Let \( S_i \) be the number of visits to state 0 in the \( i \)-th training sequence; the total number of visits then is \( S = \sum_{i=1}^{n} S_i \), with the \( S_i \) independent. Independent of \( p_0 \) and \( p_1 \) we have \( 0 \leq S_i \leq l - 1 \). We can write

\[
P(E_2) = P(S < (\pi_0 - \epsilon)(m - n) \lor m - l - S < (1 - \pi_0 - \epsilon)(m - n))
\]

\[
= P(S < (\pi_0 - \epsilon)(m - n)) + P((\pi_0 + \epsilon)(m - n) < S)
\]

Since we know the range of the \( S_i \) and they are independent, we can conveniently use Hoeffding’s inequality [26].

\[
P(S < (\pi_0 - \epsilon)(m - n)) = P\left(\frac{1}{n}(S - \pi_0(m - n)) < -\epsilon(l - 1)\right)
\]

\[
\leq \exp\left(-2\frac{n\epsilon^2(l - 1)^2}{(l - 1)^2}\right)
\]

The other probability in (42) is bound similarly.

**Theorem 3.** Consider a binary Markov chain. Assume that the training consists of a set of sequences, so that both the size of the set and the length of the sequences approach infinity. For the estimator (12), with \( \alpha = \alpha_0 \) (6) we get

\[
R_i^+(m) = \frac{2\alpha_0}{m \ln 2} + o\left(\frac{1}{m}\right)
\]

(43)
while a lower bound is
\[ R^+_i(m) \geq \frac{1}{m \ln 2} + o\left(\frac{1}{m}\right) \] (44)

**Proof.** We use the genie-inhibited estimator, so that the estimator always uses exactly \( m \) samples to estimate \( p_i \). Whenever \( E_2 \) happens, we add a penalty of 1 to the codelength and thereby get an upper bound. So,
\[
\lim_{m \to \infty} mR^+_i(m) = \lim_{m \to \infty} m \sup_{p_0, p_1} E \left[ \pi_0 D(p_0 || \hat{p}_0) + \pi_1 D(p_1 || \hat{p}_1) \right]
\leq \pi_0 \lim_{m \to \infty} \sup_{p_0} m \frac{m_0}{m_0} E \left[ D(p_0 || \hat{p}_0) \right]
+ \pi_1 \lim_{m \to \infty} \sup_{p_1} m \frac{m_1}{m_1} E \left[ D(p_1 || \hat{p}_1) \right]
+ \lim_{m \to \infty} mP(E_2)
\leq \lim_{m \to \infty} \left( \pi_0 \frac{1}{\pi_0 - \epsilon} \right) \left( 1 - \frac{1}{\delta} \right) \sup_{p_0} E \left[ D(p_0 || \hat{p}_0) \right]
+ \pi_1 \lim_{m \to \infty} \left( \pi_1 - \epsilon \right) \left( 1 - \frac{1}{\delta} \right) \sup_{p_1} E \left[ D(p_1 || \hat{p}_1) \right]
+ \lim_{m \to \infty} 2m \exp(-2n\epsilon^2)
= 2\alpha_0
\] (45)

The condition for the first two terms in (45) to converge to \( \alpha_0 \) is just that \( l \to \infty \) and \( \epsilon \to 0 \); there is no requirement on the rate of convergence. The condition for the last term to converge to zero is just that \( n \to \infty \) and that \( \epsilon \) does not converge to zero too fast. We can always choose a suitable \( \epsilon \) to satisfy this.

For the converse, we use the idealized estimator
\[
\lim_{m \to \infty} mR(m) = \lim_{m \to \infty} \inf_{m_0, p_0, p_1} m \sup_{p_0, p_1} E \left[ \pi_0 D(p_0 || \hat{p}_0) + \pi_1 D(p_1 || \hat{p}_1) \right]
\geq \inf \sup_{m_0, p_0} \left\{ \lim_{m \to \infty} m \sup_{p_0} \frac{m}{m_0} E \left[ D(p_0 || \hat{p}_0) \right] \right\}
+ \lim_{m \to \infty} \sup_{p_1} \frac{m}{m_1} E \left[ D(p_1 || \hat{p}_1) \right]
\geq \frac{1}{2} \inf \sup_{\pi_0} \pi_0 + \frac{1 - \pi_0}{1 - \pi_0}
\] (47)

where \( \hat{p}_0 \) stands for \( \frac{m_0}{m} \). The last inequality is due to [18, Theorem 2]. The minimax problem in (47) is easily solved through differentiation, with the result that the minimax solution is \( \hat{\pi}_0 = \pi_0 = \frac{1}{2} \), which gives \( \lim_{m \to \infty} mR(m) \geq 1 \).

The result could potentially be improved by considering the modified estimator from [21] that resulted in (7).

**Theorem 4.** Consider a binary Markov chain. Assume that the training consists of a set of sequences, so that both the size of the set and the length of the sequences approach infinity. Using the estimator from Theorem 7, the following decay is achievable
\[
a(m, P_e) = 2b(P_e) \frac{Q^{-1}(1 - \sqrt{1 - P_e})}{2m \ln 2} + o\left(\frac{1}{m}\right)
\] (48)

This is achievable for
\[
\frac{1}{6} Q^{-1}(1 - \sqrt{1 - P_e})^2 - 1 \leq a \leq \frac{1}{6} Q^{-1}(1 - \sqrt{1 - P_e})^2 + 1
\]
Theorem 5. A lower bound is

\[ E(m) \leq \sup_{p_0, p_1} (P(E_1) + P(E_2)) \]

Of course, the addition of extra artificial data can decrease \( P(E_1) \), but whenever artificial data is added \( E_2 \) happens, and the total error probability is not decreased. Here

\[
P(E_1) = 1 - P(\pi_0 D(p_0 \| \hat{p}_0) + \pi_1 D(p_1 \| \hat{p}_1) \leq a) \\
\leq 1 - P(D(p_0 \| \hat{p}_0) \leq \frac{a}{2\pi_0} \wedge D(p_1 \| \hat{p}_1) \leq \frac{a}{2\pi_1}) \\
= 1 - P(D(p_0 \| \hat{p}_0) \leq \frac{a}{2\pi_0}) P(D(p_1 \| \hat{p}_1) \leq \frac{a}{2\pi_1})
\]

because the random variables \( \hat{p}_0 \) and \( \hat{p}_1 \) are independent with the way the (augmented) data set is generated. We now require

\[
P\left(D(p_i \| \hat{p}_i) \geq \frac{a}{2\pi_i}\right) \leq 1 - \sqrt{1 - Pe + P(E_2)}
\]

Notice that by construction, \( \hat{p}_i \) has exactly the same distribution as \( \hat{p} \) in Theorem 1 except based on \( m_i \) samples instead of \( m \). By Theorem 1 (49) is satisfied if

\[
\frac{a}{2\pi_i} \geq \frac{b(Pe)Q^{-1}(1 - \sqrt{1 - Pe + P(E_2)})/2}{m_i \ln 2} + o\left(\frac{1}{m}\right).
\]

With \( m_i \) given by (40) and \( P(E_2) \) bounded by Lemma 2 as long as both \( n, l \to \infty \), we can let \( \epsilon \) converge to 0 sufficiently slowly so that we get (48).

\[ \Box \]

Theorem 5. A lower bound is

\[
a(m, Pe) \geq \frac{F_{\chi^2}^{-1}(1 - Pe)}{2m \ln 2} + o\left(\frac{1}{m}\right)
\]

where \( F_{\chi^2} \) is the CDF for a \( \chi^2 \)-distribution with two degrees of freedom.

Proof. The proof follows closely the proof of the lower bound in Theorem 1 and we only provide the outline here. We do the lower bound for the CLT regime, and we use (18) to lower bound relative entropy,

\[
\pi_0 D(p_0 \| \hat{p}_0) + \pi_1 D(p_1 \| \hat{p}_1) \geq \frac{2}{\ln 2} \left( \pi_0 (\hat{p}_0 - p_0)^2 + \pi_1 (\hat{p}_1 - p_1)^2 \right)
\]

We have \( \hat{p}_i = f_i(\hat{p}_0) \), which we assume is invertible; we write \( \hat{p}_i = f^{-1}(\hat{p}_i) = \hat{p}_i + g_i(m)(\hat{p}_i) \). Let

\[
S_a = \left\{ (\hat{p}_0, \hat{p}_1) : \frac{2}{\ln 2} \left( \pi_0 (\hat{p}_0 - p_0)^2 + \pi_1 (\hat{p}_1 - p_1)^2 \right) \leq a \right\}
\]

which is an ellipsoid centered at \( (p_0, p_1) \). Consider the set of points satisfying

\[
(\sqrt{m}(\hat{p}_0 - p_0), \sqrt{m}(\hat{p}_1 - p_1)) \in \sqrt{m}(S_a - (p_0, p_1)) + \sqrt{m}g_m(S_a)
\]

Here \( \sqrt{m}(\hat{p}_i - p_i) \) converge to independent Gaussians by the central limit theorem. To achieve a given \( Pe \) we must then have a decrease as \( \frac{1}{m} \), and \( S_a \) is a shrinking ellipsoid. As in the proof of Theorem 1 we see that \( \sqrt{m}g_m(S_a) \) converges to a single point, \( b \). The goal is to minimize \( a \) while still having
$P(S_a) \geq 1 - P_e$. It is easily seen that this is achieved for $b = 0$. Finally the worst case over $p_0, p_1$ is for $p_0 = p_1 = \frac{1}{2}$ while the best case is $m = \pi, m$. We end up with analyzing the symmetric case, $\hat{p}_i - p_i \sim N(0, \frac{1}{2m})$, so that

$$2m \ln 2 \frac{1}{\ln 2} \left( \frac{1}{2}(\hat{p}_0 - p_0)^2 + \frac{1}{2}(\hat{p}_1 - p_1)^2 \right) \sim \chi^2_2$$

and

$$a(m, P_e) \geq \frac{F_{\chi^2_2}^{-1}(1 - P_e)}{2m \ln 2}$$

As opposed to the IID case, Theorem [1] the upper and lower bounds are not tight as $P_e \to 0$. There is a factor about 2 between the bounds. Both bounds require evaluations of the probability of a set $\{\hat{p}_0, \hat{p}_1 : \pi_0 D(p_0||\hat{p}_0) + \pi_1 D(p_1||\hat{p}_1) \leq a\}$. The achievable bound bounds this by the probability of a square, while the converse uses a circle, and the gap is due to this difference. Fig. [2] shows the different bounds. The achievable bounds indicates that the Markov chain requires more than twice as many training samples as the iid case; but the lower bound shows that hardly any increase in samples is needed (though at least it proves that some more samples are required).

However, our bottom-line comparison was with universal source coding. The redundancy of universal source coding of a Markov chain with 2 states is about $R^u_t \approx \log l$ [27], a factor 2 increase over IID sources. For the achievable rate we also have about a factor 2 increase, and therefore approximately

$$m \geq \frac{Q^{-1}(P_e/2)^2}{2 \ln 2} \frac{l}{\log l}$$

the same as (35). Thus no more samples are required than for the IID case. On the other hand, if we go with the lower bound, the factor for training is closer to 1, and the conclusion is therefore that only half the number of samples is required to beat universal coding for Markov chains compared to the IID case: it is even easier to learn Markov chains than IID sources! The author does not really have a conjecture on whether the upper or lower bound is tighter.

Figure 2. Plot of the gap between the IID lower bound and the Markov bounds.

Finally, the condition for achievability in both Theorems [3 and 4] is just that both the number of training sequences $n$ and their length $l$ approach infinity, but it does not matter how. One would think that there would be an optimum relationship between $n$ and $l$, but obviously that does not affect the performance to the first order.
IV. CONCLUSIONS

The central question of this paper can be thought of as: how much training is required to beat universal source coding? The answer for both IID sources and Markov chains is: not many. To code a sequence of length \( l \) the number of training samples is proportional to \( \frac{l}{\log 7} \). This optimistic conclusion is totally opposite to the pessimistic conclusion of [15]. The reason is due to the viewpoint – and perhaps that we so far only consider very simple sources. While [15] focuses on approaching entropy rate, we just want to beat the redundancy of universal source coding. Additionally, [15] considers learning to be that of building a dictionary, inspired by Lempel-Ziv coding [1, 2]. However, the exceptional performance of modern machine learning can be seen as being achieved through learning soft information. This is also how we approach learning here, and the coding is more similar to the CTW algorithm of Willems [28].

The paper also shows that it is essential to have multiple training sequences for Markov chains, which is different from universal prediction.

Natural generalization of the result is to larger alphabet sizes and Markov chains with more than two states. The most interesting generalization is to finite state machines (FSM) as in [27]. FSM are much more realistic of real-world sources, and potentially they might not be so easy to learn.

Another interesting generalization would be to the large deviations regime. In this case \( \alpha \) would be fixed and the question then is how \( P_e \) decreases with \( m \). This seems to be more difficult than the moderate deviations considered here. One thing we can already predict from the results here is that in the large deviation regime the "add \( \alpha \)" estimator (12) is no longer suitable. Namely, from (14) it can be seen that the optimum \( \alpha \) depends on \( P_e \), which again depends on \( m \) for large deviations. Thus, \( \alpha \) must also be a function of \( m \). In fact, from some initial numerical observations, it seems the estimator (11) with \( \beta \) constant works much better.

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