CONCENTRATION OF THE MULTINOMIAL IN KULLBACK–LEIBLER DIVERGENCE NEAR THE RATIO OF ALPHABET AND SAMPLE SIZES

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Abstract. We bound the moment generating function of the Kullback–Leibler divergence between the empirical distribution of independent samples from a distribution over a finite alphabet (e.g. a multinomial distribution) and the underlying distribution via a simple reduction to the case of a binary alphabet (e.g. a binomial distribution). The resulting concentration inequality becomes meaningful (less than 1) when the deviation \( \varepsilon \) is a constant factor larger than the ratio \((k - 1)/n\) for \( k \) the alphabet size and \( n \) the number of samples, whereas the standard method of types bound requires \( \varepsilon > (k - 1)/n \cdot \log(1 + n/(k - 1)) \).

1. Introduction

A basic problem in statistics is to understand the convergence of an empirical distribution of independent samples from a distribution \( P \) to the underlying distribution. In this work, we derive concentration bounds for the specific case of this problem of analyzing the KL-divergence (relative entropy) between the empirical distribution of \( n \) samples drawn from a distribution \( P \) over a finite alphabet of size \( k \) and \( P \) itself:

Definition 1.1. Let \( X = (X_1, \ldots, X_k) \) be distributed according to a multinomial distribution with \( n \) samples and probabilities \( P = (p_1, \ldots, p_k) \), and define

\[
\hat{V}_{n,k,P} \overset{\text{def}}{=} \text{KL}((X_1/n, \ldots, X_k/n) \| (p_1, \ldots, p_k))
\]

where

\[
\text{KL}((q_1, \ldots, q_k) \| (p_1, \ldots, p_k)) \overset{\text{def}}{=} \sum_{i=1}^{k} q_i \log \frac{q_i}{p_i}
\]

is the Kullback–Leibler (KL) divergence or relative entropy between two probability distributions on a finite set \( \{1, \ldots, k\} \) (represented as probability mass functions), and \( \log \) is in the natural base (as are all logarithms and exponentials in this work).

We seek upper bounds on \( \Pr[\hat{V}_{n,k,P} > \varepsilon] \) which ideally are meaningful (less than 1) when \( \varepsilon \) is close to \((k - 1)/n\), since Paninski [Pan02] showed that \( \mathbb{E}[\hat{V}_{n,k,P}] \leq \log(1 + k - 1/n) \leq \frac{k - 1}{n} \), and conversely Jiao, Venkat, Han, and Weissman [JVHW17] showed that for \( P \) the uniform distribution and large enough \( n \) that \( \mathbb{E}[\hat{V}_{n,k,U_k}] \geq \frac{k - 1}{n} \cdot \frac{1}{2} \). Antos and Kontoyiannis [AK01]

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used McDiarmid’s bounded differences inequality [McD89] to give a concentration bound for the empirical distribution, in which the case of the uniform distribution implies the bound
\[
\Pr \left[ \left| \hat{V}_{n,k,p} - \mathbb{E} \hat{V}_{n,k,U_k} \right| \geq \varepsilon \right] \leq 2e^{-n\varepsilon^2/(2\log^2 n)}.
\]
This bound has the advantage of providing subgaussian concentration around the expectation, but for the case of small \( \varepsilon < 1 \) it is preferable to have a bound with linear dependence on \( \varepsilon \). Unfortunately, existing tail bounds which decay like \( e^{-n\varepsilon} \) are not, in the regime of parameters where \( n \gg k \), meaningful for \( \varepsilon \) close to \( (k - 1)/n \). For example, the standard tail bound based on the method of types (e.g., [CS14 Corollary 2.1]) states
\[
(1.1) \quad \Pr \left[ \left| \hat{V}_{n,k,p} - \mathbb{E} \hat{V}_{n,k,U_k} \right| \geq \varepsilon \right] \leq e^{-n\varepsilon} \cdot \left( \frac{n + k - 1}{k - 1} \right),
\]
which is meaningful only for \( \varepsilon > \frac{1}{n} \cdot \log \left( \frac{n + k - 1}{k - 1} \right) \geq \frac{k - 1}{n} \cdot \log \left( 1 + \frac{n}{k - 1} \right) \), which is off by a factor of order \( \log \left( 1 + \frac{n}{k - 1} \right) \). A recent bound due to Mardia, Jiao, Tánczos, Nowak, and Weissman [MJT+18] improved on the method of types bound for all settings of \( k \) and \( n \), but for \( 3 < k \leq \frac{e}{2\pi} \cdot n \) still requires \( \varepsilon > \frac{k}{n} \cdot \log \left( \frac{e\pi}{2\pi k} \right) > \frac{k - 1}{n} \cdot \log \left( 1 + \frac{n - 1}{k} \right) / 2 \), which again has dependence on \( \log \left( 1 + \frac{n - 1}{k} \right) \).

The main result of this work is the following tail bound without this extra dependence on \( \log \left( 1 + \frac{n - 1}{k} \right) \):

**Theorem 1.2.** Let \( \hat{V}_{n,k,p} \) be as in Definition 1.1. Then for all \( \varepsilon > \frac{k - 1}{n} \cdot (1 + \log 2) \), it holds that
\[
\Pr \left[ \left| \hat{V}_{n,k,p} - \mathbb{E} \hat{V}_{n,k,U_k} \right| \geq \varepsilon \right] \leq 2e^{-\varepsilon} \cdot \left( \frac{\varepsilon n}{k - 1} - \log 2 \right) \cdot \left( \frac{1}{2} \right)^{k - 1}.
\]

In particular, if \( k \) is a constant or even a small polynomial of \( n \), e.g. \( k = n^{0.99} \), the above bound is meaningful for \( \varepsilon \) smaller than what is needed for the method of types bound or the bound of [MJT+18] by a factor of order \( \log(n) \). However, Theorem 1.2 has slightly worse dependence on \( \varepsilon \) than the other bounds, so for example it is better than the method of types bound if and only if
\[
(1.2) \quad \frac{k - 1}{n} \cdot (\log 2 + 1) < \varepsilon < \frac{k - 1}{n} \cdot \left( \log 2 + \frac{1}{2} \cdot \frac{1}{2^{k - 1}} \cdot \left( \frac{n + k - 1}{k - 1} \right)^{k - 1} \right).
\]

Since \( e^{k - 1} \cdot \left( 1 + \frac{n}{k - 1} \right)^{k - 1} \geq \left( n^{k - 1} \right)^{k - 1} \geq 1 + \frac{n}{k - 1} \), we summarize Eq. (1.2) in the looser but easier to understand Table 1.

| Theorem 1.2 better | Method of types better |
|-------------------|-----------------------|
| \( \frac{k - 1}{n} \cdot (\log 2 + 1) < \varepsilon < \frac{k - 1}{n} \cdot \left( \log 2 + \frac{1}{2} \cdot \left( 1 + \frac{n}{k - 1} \right) \right) \) | \( \varepsilon > \frac{k - 1}{n} \cdot \left( \log 2 + \frac{1}{2} \cdot \left( 1 + \frac{n}{k - 1} \right) \right) \) |

**Table 1.** Comparison of Theorem 1.2 and the method of types bound Eq. (1.1).
the size of the alphabet. In this regime, we can also compare to the “interpretable” upper bound of [MJT+18 Theorem 3], to see that Theorem 1.2 is better if

$$\frac{k-1}{n} \cdot (\log 2 + 1) < \varepsilon < \frac{k-1}{n} \cdot \left( \log 2 + \left( \frac{6e^2}{\pi^{3/2}} \sqrt{\frac{en}{2\pi k}} \right)^{1/(k-1)} \right),$$

so that in particular it suffices to have

$$\frac{k-1}{n} \cdot (\log 2 + 1) < \varepsilon < \frac{k-1}{n} \cdot \left( \log 2 + \sqrt{\frac{n}{k}} \right).$$

We prove Theorem 1.2 by bounding the moment generating function of $\hat{V}_{n,k,P}$:

**Theorem 1.3.** Let $\hat{V}_{n,k,P}$ be as in Definition 1.1. Then for all $0 \leq t < n$ it holds that

$$E\left[ \exp\left( t \cdot \hat{V}_{n,k,P} \right) \right] \leq \left( \frac{2t/n}{1-t/n} \right)^{k-1}.$$

Perhaps surprisingly, to establish Theorem 1.3 we need only basic properties of conditional expectation and Hoeffding’s inequality [Hoe63].

2. **Reducing the Multinomial to the Binomial**

To prove Theorem 1.3 we show the moment generating function of $\hat{V}_{n,k,P}$ can be bounded in terms of binomial KL $\hat{V}_{n,2,P}$ moment generating function bounds of a specific form. Formally:

**Definition 2.1.** A function $f : [0, 1) \to \mathbb{R}$ is a sample-independent MGF bound for the binomial KL if for every positive integer $n$, real $t \in [0, n)$, and $p \in [0, 1]$ it holds that

$$E\left[ \exp\left( t \cdot \hat{V}_{n,2,(p,1-p)} \right) \right] \leq f(t/n).$$

**Proposition 2.2.** Let $P = (p_1, \ldots, p_k)$ be a distribution on a set of size $k$ for $k \geq 2$. Then for every sample-independent MGF bound for the binomial KL $f : [0, 1) \to \mathbb{R}$ and $0 \leq t < n$, the moment generating function of $\hat{V}_{n,k,P}$ satisfies

$$E\left[ \exp\left( t \cdot \hat{V}_{n,k,P} \right) \right] \leq f(t/n)^{k-1}.$$

**Proof.** This is a simple induction on $k$. The base case $k = 2$ holds by definition of sample-independent MGF bound for the binomial KL.

For the inductive step, we compute conditioned on the value of $X_k$. Note that if $p_k = 1$ then the inductive step is trivial since $\hat{V}_{n,k,P} = 0$ with probability 1, so assume that $p_k < 1$. For each $i \in \{1, \ldots, k-1\}$ define $p'_i = p_i/(1-p_k)$, so that conditioned on $X_k = m$, the variables $(X_1, \ldots, X_{k-1})$ are distributed multinomially with $n - m$ samples and probabilities
Remark where we treat the second term as position of the multinomial KL to inductively bound the (non-exponential) moments. By definition of a sample-independent MGF bound for the binomial KL, the second term is upper bound if

\[ \mu = e^{-t/n} \sum_{i=1}^{k-1} X_i \log \frac{(n-X_k)/n}{p'_i} \]

\[ = \text{KL} \left( \frac{X_k}{n-\hat{X}_k}, \ldots, \frac{X_{k-1}}{n-\hat{X}_k} \right) \mid (p'_1, \ldots, p'_{k-1}) \]

where we treat the second term as 0 if \( X_k = n \). Thus for every \( 0 \leq t < n \) we have

\[ E \left[ \exp \left( t \cdot \text{KL} \left( (X_1,n, \ldots, X_k/n) \mid (p_1, \ldots, p_k) \right) \right) \right] \]

\[ = E \left[ E \left[ \exp \left( t \cdot \text{KL} \left( (X_1, n, \ldots, X_k/n) \mid (p_1, \ldots, p_k) \right) \right) \mid X_k \right] \right] \]

\[ = \exp \left( t \cdot \text{KL} \left( (X_k/n, 1 - X_k/n) \mid (p_k, 1 - p_k) \right) \right) \]

\[ \cdot E \left[ \exp \left( t \cdot \frac{n-X_k}{n} \cdot \text{KL} \left( \left( \frac{X_1}{n-X_k}, \ldots, \frac{X_{k-1}}{n-X_k} \right) \mid (p'_1, \ldots, p'_{k-1}) \right) \right) \mid X_k \right] \].

Since \( 0 \leq t \cdot \frac{n-X_k}{n} < n - X_k \), the inductive hypothesis for \( \tilde{V}_{n-k,k-1, (p'_1, \ldots, p'_{k-1})} \) implies the upper bound

\[ \leq E \left[ \exp \left( t \cdot \text{KL} \left( (X_k/n, 1 - X_k/n) \mid (p_k, 1 - p_k) \right) \right) \cdot f \left( \frac{t(n-X_k)/n}{n-X_k} \right)^{k-2} \right] \]

\[ = f(t/n)^{k-2} \cdot E \left[ \exp \left( t \cdot \text{KL} \left( (X_k/n, 1 - X_k/n) \mid (p_k, 1 - p_k) \right) \right) \right] \].

By definition of a sample-independent MGF bound for the binomial KL, the second term is at most \( f(t/n) \), so we get a bound of \( f(t/n)^{k-1} \) as desired.

\[ \square \]

Remark 2.3. Mardia, Jiao, Tánzos, Nowak, and Weissman \[MJT^{+}18 \] use the same decomposition of the multinomial KL to inductively bound the (non-exponential) moments.

3. Bounding the Binomial

It remains to give a sample-independent MGF bound for the binomial KL:
Lemma 3.1. The function
\[ f(x) = \frac{2^x}{1 - x} \]
is a sample-independent MGF bound for the binomial KL.

Before giving the proof, for convenience we make the following definition:

Definition 3.2. For real \( p, q \in [0, 1] \), we abbreviate \( \text{BernKL}(p \parallel q) \) defined as \( \text{KL}( (p, 1 - p) \parallel (q, 1 - q)) \).

Proof of Lemma 3.1. Hoeffding’s inequality [Hoe63] states that for \( B \sim \text{Binomial}(n, p) \) and real \( k \geq np \) that \( \Pr[B \geq k] \leq \exp(-n \cdot \text{BernKL}(k/n \parallel p)) \), and likewise for \( k \leq np \) and \( \Pr[B \leq k] \). In particular, this implies
\[ \Pr[\text{BernKL}(B/n \parallel p) \geq \varepsilon] \leq \Pr[\text{BernKL}(B/n \parallel p) \geq \varepsilon \land B \geq np] + \Pr[\text{BernKL}(B/n \parallel p) \geq \varepsilon \land B \leq np] \]
\[ \leq 2e^{-n\varepsilon} \]
by looking at the upper and lower inverses of BernKL (see [MJT+18, Lemma 8] for another proof). Hence, for \( 0 \leq t < n \) we have
\[ \mathbb{E}[\exp(t \cdot \text{BernKL}(B/n \parallel p))] = \int_0^\infty \Pr[\exp(t \cdot \text{BernKL}(B/n \parallel p)) > x] \, dx \]
\[ = \int_0^\infty \Pr\left[\text{BernKL}(B/n \parallel p) > \frac{\log x}{t}\right] \, dx \]
\[ \leq \int_0^\infty \min\{1, 2e^{-n\log x/t}\} \, dx \]
\[ = \int_0^{2^{t/n}} 1 \, dx + \int_{2^{t/n}}^\infty \frac{2}{x^{n/t}} \, dx \]
\[ = \frac{2^{t/n}}{1 - t/n}. \]

Together, Proposition 2.2 and Lemma 3.1 imply our moment generating function bound (Theorem 1.3), and thus a Chernoff bound implies our tail bound:

Proof of Theorem 1.2. By Theorem 1.3, we know for every \( x \in [0, 1) \) that the moment generating function \( \mathbb{E}[\exp(n x \cdot \hat{V}_{n,k,P})] \) is at most \( \left( \frac{2^x}{1 - x} \right)^{k-1} \), so by a Chernoff bound
\[ \Pr\left[\hat{V}_{n,k,P} > \varepsilon\right] \leq \inf_{x \in [0,1)} \exp(-n \varepsilon \cdot x) \cdot \left( \frac{2^x}{1 - x} \right)^{k-1}. \]
The result follows by making the optimal choice
\[ x = 1 - \frac{1}{(\varepsilon n) / (k - 1) - \log 2} \]
when \( \varepsilon > \frac{k-1}{n} \cdot (1 + \log 2) \).

We believe that Lemma 3.1 can be improved, as numerical evidence suggests the following conjecture:
Conjecture 3.3. The functions
\[ f(x) = \frac{2}{\sqrt{1 - x}} - 1 \leq g(x) = \frac{1}{1 - x} \]
are sample-independent MGF bounds for the binomial KL.

Remark 3.4. Under the above conjectures, we would obtain via Proposition 2.2 and a Chernoff bound that
\[
\Pr[\hat{V}_{n,k,p} > \varepsilon] \leq e^{-n\varepsilon} \cdot \left( e \cdot \left( 2 \frac{\varepsilon n}{k-1} - 1 \right) \right)^{k-1} \quad \text{(under the stronger conjecture)}
\]
\[
\leq e^{-n\varepsilon} \cdot \left( e \cdot \frac{\varepsilon n}{k-1} \right)^{k-1} \quad \text{(under the weaker conjecture)}
\]
for all \( \varepsilon > (k-1)/n \).

The stronger of the two conjectures above is motivated by the following conjecture, which looks at a single branch of the KL-divergence:

Conjecture 3.5. Letting
\[
\text{BernKL}_>(p \parallel q) \overset{\text{def}}{=} \begin{cases} 
0 & p \leq q \\
\text{KL}((p, 1-p) \parallel (q, 1-q)) & p > q
\end{cases}
\]
it holds for every positive integer \( n \), real \( t \in [0,n) \), and \( p \in [0,1] \) that
\[
\mathbb{E}\left[ \exp\left( t \cdot \text{BernKL}_>(B/n \parallel p) \right) \right] \leq \frac{1}{\sqrt{1 - t/n}}
\]
where \( B \sim \text{Binomial}(n,p) \).

Remark 3.6. Note that \( \frac{1}{\sqrt{1 - t/n}} \) is the moment generating function of \( \chi_1^2/(2n) \).

Remark 3.7. We believe the results (or techniques) of Zubkov and Serov [ZS13] and Harremoës [Har17] strengthening Hoeffding’s inequality may be of use in proving these conjectures.

Proof of Conjecture 3.3 given Conjecture 3.5 We have that
\[
\text{KL}((p, 1-p) \parallel (q, 1-q)) = \text{BernKL}_>(p \parallel q) + \text{BernKL}_>(1-p \parallel 1-q)
\]
so for every \( k \in \{0,1,\ldots,n\} \)
\[
\exp\left( t \cdot \text{KL}(k/n, 1-k/n \parallel (p, 1-p)) \right)
= \exp\left( t \cdot \text{BernKL}_>(k/n \parallel p) \right) \cdot \exp\left( t \cdot \text{BernKL}_>(1-k/n \parallel 1-p) \right).
\]
Letting \( x = \exp\left( t \cdot \text{BernKL}_>(k/n \parallel p) \right) \) and \( y = \exp\left( t \cdot \text{BernKL}_>(1-k/n \parallel 1-p) \right) \), we have that at least one of \( x \) and \( y \) is equal to 1, so that
\[
xy = (1 + (x - 1))(1 + (y - 1)) = 1 + (x - 1) + (y - 1) + (x - 1)(y - 1) = x + y - 1,
\]
and thus by taking expectations over \( k = B \) for \( B \sim \text{Binomial}(n,p) \), we get
\[
\mathbb{E}[\exp(t \cdot \text{BernKL}(B/n \parallel p))] = \mathbb{E}[\exp(t \cdot \text{BernKL}_>(B/n \parallel p))] + \mathbb{E}[\exp(t \cdot \text{BernKL}_>(1-B/n \parallel 1-p))] - 1.
\]
We conclude by bounding both terms using Conjecture 3.5 since \( n - B \) is distributed as Binomial\((n, 1 - p)\).

\[\square\]

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