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1 Definitions

In this TED talk, we will talk about the relation between Kullback-Leibler divergence and the total variation distance between probability distributions. We will focus on **discrete** probability distributions only. Let's start with some definitions and assumed theorems first:

Definition 1.1. S is a sample space, $\mathcal{A} = 2^S$. A probability distribution $P : \mathcal{A} \to [0, 1]$ is a probability distribution. P satisfies Kolmogorov axioms of probability.

For $s \in S$, we also use the shorthand notation $P(s) := P(\{s\})$.

Definition 1.2. The Kullback-Leibler divergence between two probability distributions P(x) and Q(x) from discrete probability spaces defined over the same S is

$$D_{KL}(P||Q) = \sum_{x \in S} P(x) \log \frac{P(x)}{Q(x)}.$$
(1)

Definition 1.3. The Manhattan distance $(L_1 \text{ metric})$ between two probability distributions P(x) and Q(x) from discrete probability spaces defined over the same S is

$$||P - Q||_1 = \sum_{x \in S} |P(x) - Q(x)|.$$
(2)

Definition 1.4. The total variation distance between two probability distributions P(x) and Q(x) from discrete probability spaces defined over the same S is

$$\delta(P,Q) = \max_{A \in 2^{S}} |P(A) - Q(A)|.$$
(3)

Theorem 1.5. Jensen's inequality.

For a convex function f, and reals $p_1, \ldots, p_n \ge 0$ such that $\sum_{i=1}^n p_i = 1$ it holds that:

$$f\left(\sum_{i=1}^{n} p_i x_i\right) \le \sum_{i=1}^{n} p_i f(x_i) \tag{4}$$

2 Lower Bound

Theorem 2.1. Pinsker's inequality. For two probability distributions P(x) and Q(x) from discrete probability spaces defined over the same S, it holds that

$$||P - Q||_1 \le \sqrt{2} \operatorname{D}_{\mathrm{KL}}(P||Q).$$

The equivalent inequality is that

$$D_{KL}(P||Q) \ge \frac{1}{2}||P - Q||_1^2.$$

Proof. Bernoulli distributions case.

Let's denote by P and Q Bernoulli distribution over $S = \{0, 1\}$. Also, denote:

$$p = P(0), 1 - p = P(1)$$

$$q = Q(0), 1 - q = Q(1)$$

We can see that

$$||P - Q||_1 = |p - q| + |1 - p - 1 + q| = 2 \cdot |p - q|$$
$$||P - Q||_1^2 = 4(p - q)^2$$

Let's define $f(p,q) = D_{KL}(P||Q) - \frac{1}{2}||P - Q||_1^2$. We will analyse the behaviour of the function using basic calculus.

$$\begin{split} f(p,q) &= p \log \frac{p}{q} + (1-p) \log \frac{1-p}{1-q} - 2(p-q)^2 \\ \frac{\partial f}{\partial q} &= p \cdot \frac{q}{p} \cdot \frac{-p}{q^2} + (1-p) \cdot \frac{1-q}{1-p} \cdot (1-p) \frac{-1}{(1-q)^2} \cdot (-1) - 4(p-q) \cdot (-1) \\ &= -\frac{p}{q} + \frac{1-p}{1-q} + 4(p-q) \\ &= \frac{-p+pq+q-pq}{q(1-q)} - 4(q-p) \\ &= (q-p) \left[\frac{1}{q(1-q)} - 4 \right] \end{split}$$

We see that with $q \neq \frac{1}{2}$, the sign of the partial derivative depends only on the sign of q - p. Therefore, $\frac{\partial f}{\partial q}$ is negative for q < p, positive for q > p and 0 for q = p. That means that for $q \neq \frac{1}{2}$, q = p is the minimum of f(p,q).

$$f(p,p) = p \log \frac{p}{p} + (1-p) \log \frac{1-p}{1-p} - 2(p-p)^2$$

= 0.

That means that for $q \neq \frac{1}{2}$, f(p,q) is non-negative and the Pinsker's inequality holds. We now analyze

$$\begin{split} g(p) &= f\left(p, \frac{1}{2}\right) = p \cdot \log(2p) + (1-p) \cdot \log(2-2p) - 2 \cdot \left(p - \frac{1}{2}\right)^2 \\ g'(p) &= \log(2p) + p \cdot \frac{1}{2p} \cdot 2 + (-1) \cdot \log(2-2p) + (1-p) \cdot \frac{1}{2-2p} \cdot (-2) - 4 \cdot (p - \frac{1}{2}) \\ &= \log(2p) + 1 - \log(2-2p) - 1 - 4p + 2 \\ &= \log(2p) - \log(2-2p) - 4p + 2. \\ g''(p) &= \frac{1}{2p} \cdot 2 - \frac{1}{2-2p} \cdot (-2) - 4 \\ &= \frac{1}{2p} + \frac{1}{1-p} - 4 = \frac{1-p+p-4p+4p^2}{p \cdot (1-p)} \\ &= \frac{4p^2 - 4p + 1}{p - p^2} = \frac{4\left(p - \frac{1}{2}\right)^2}{p \cdot (1-p)}. \end{split}$$

For $p \in (0, 1)$, the denominator of the second derivative is always positive and therefore the sign depends only on the nominator. As the nominator is also non-negative for $p \in (0, 1)$, the second derivative is always non-negative and the first derivative is therefore a non-decreasing function.

$$g'\left(\frac{1}{2}\right) = \log 1 - \log 1 - 2 + 2 = 0$$
$$g\left(\frac{1}{2}\right) = \frac{1}{2} \cdot \log 1 + \frac{1}{2} \cdot \log 1 - 0 = 0$$
$$g(0) = 0 \cdot \log 0 + 1 \cdot \log 2 = \infty$$
$$g(1) = 1 \cdot \log 2 + 0 \cdot \log 0 = \infty$$

The figure sums up our analysis:



Therefore, the Pinsker's inequality holds for two arbitrary Bernoulli distributions. For the general case, we will need the log sum inequality and the information processing inequality:

Lemma 2.2. Log sum inequality Let $p_1, p_2, \ldots, p_n, q_1, q_2, \ldots, q_n \in \mathbb{R}^+_0$ be non-negative real numbers. Let $p = \sum_{i=1}^n p_i$ and $q = \sum_{i=1}^n q_i$. Then

$$\sum_{i=1}^{n} p_i \log \frac{p_i}{q_i} \ge p \log \frac{p}{q}.$$

Proof. Set $f(x) = x \log x$. Notice that f is a convex function. Then,

$$\sum_{i=1}^{n} p_i \log \frac{p_i}{q_i} = \sum_{i=1}^{n} p_i \frac{q_i}{q_i} \log \frac{p_i}{q_i}$$
$$= \sum_{i=1}^{n} q_i f\left(\frac{p_i}{q_i}\right)$$
$$= q \sum_{i=1}^{n} \frac{q_i}{q} f\left(\frac{p_i}{q_i}\right)$$
$$\ge q \cdot f\left(\sum_{i=1}^{n} \frac{q_i}{q} \cdot \frac{p_i}{q_i}\right)$$
$$= q \cdot f\left(\frac{1}{q} \sum_{i=1}^{n} p_i\right) = q \cdot f\left(\frac{p}{q}\right)$$
$$= q \cdot \frac{p}{q} \cdot \log \frac{p}{q}$$
$$= p \log \frac{p}{q}.$$

Lemma 2.3. Information processing inequality.

For any function $f: S \to S'$ and probability distributions $X: 2^S \to [0, 1]$ and $Y: 2^S \to [0, 1]$ defined over S, define

$$X': 2^{S'} \to [0, 1],$$

 $Y': 2^{S'} \to [0, 1].$

For every $i \in S'$, define

$$X'(i) = X(f^{-1}(i)) = \sum_{w \in f^{-1}(i)} X(w),$$

$$Y'(i) = Y(f^{-1}(i)) = \sum_{w \in f^{-1}(i)} Y(w).$$

If X' and Y' are probability distributions, then

$$D_{\mathrm{KL}}(X'||Y') \le D_{\mathrm{KL}}(X||Y).$$

Proof.

$$D_{\mathrm{KL}}(X||Y) = \sum_{w \in S} X(w) \log \frac{X(w)}{Y(w)}$$
$$= \sum_{i \in S'} \sum_{w \in f^{-1}(i)} X(w) \log \frac{X(w)}{Y(w)}$$
$$\geq \sum_{i \in S'} X'(i) \log \frac{X'(i)}{Y'(i)}$$
$$= D_{\mathrm{KL}}(X'||Y').$$

Proof. Pinsker's inequality. Given probability distributions P(x) and Q(x) from discrete probability spaces defined over the same S, define $f: S \to \{0, 1\}$

$$f(w) = \begin{cases} 1 & P(w) \le Q(w), \\ 0 & P(w) > Q(w). \end{cases}$$

Define probability distributions $P', Q' : 2^{\{0,1\}} \to [0,1]$ for $i \in \{0,1\}$ as

$$P'(i) = P(f^{-1}(i)) = \sum_{w \in f^{-1}(i)} P(w),$$
$$Q'(i) = Q(f^{-1}(i)) = \sum_{w \in f^{-1}(i)} Q(w),$$
$$P'(0) = \sum_{\{w \in S \mid P(w) > Q(w)\}} P(w),$$
$$Q'(0) = \sum_{\{w \in S \mid P(w) > Q(w)\}} Q(w),$$
$$P'(1) = \sum_{\{w \in S \mid P(w) \le Q(w)\}} P(w),$$
$$Q'(1) = \sum_{\{w \in S \mid P(w) \le Q(w)\}} Q(w).$$

From this follows that P'(0) > Q'(0) and $P'(1) \le Q'(1)$.

As P' and Q' are Bernoulli distributions, we know that $D_{KL}(P'||Q') \ge \frac{1}{2}||P' - Q'||_1^2$ by Pinsker's inequality for Bernoulli distributions.

Also,

$$\begin{split} ||P - Q||_1 &= \sum_{w \in S} |P(w) - Q(w)| \\ &= \sum_{w \in f^{-1}(0)} (P(w) - Q(w)) + \sum_{w \in f^{-1}(1)} (Q(w) - P(w)) \\ &= P'(0) - Q'(0) + Q'(1) - P'(1) \\ &= |P'(0) - Q'(0)| + |P'(1) - Q'(1)| \\ &= ||P' - Q'||_1. \end{split}$$

Therefore, $D_{KL}(P'||Q') \ge \frac{1}{2}||P - Q||_1^2$.

By information processing inequality, we know that

$$D_{\mathrm{KL}}(P'||Q') \le D_{\mathrm{KL}}(P||Q).$$

And that is all, folks!

$$D_{KL}(P||Q) \ge D_{KL}(P'||Q') \ge \frac{1}{2}||P' - Q'||_1^2 = \frac{1}{2}||P - Q||_1^2.$$

3 Upper Bound

There does not exist such a nice lower bound for KL divergence for a simple reason.

3.1 A counterexample

Theorem 3.1. Kullback-Leibler divergence is not upper bounded by the L_1 metric. Formally, for every $\varepsilon > 0$, there exist probability distributions P_{ε} and Q such that:

$$||P - Q||_1 \le \varepsilon$$
, but $D_{KL}(P||Q) = \infty$.

Proof. Define P(x) and Q as

$$S = \{a, b\}$$

$$Q(a) = 0, Q(b) = 1$$

$$P_{\varepsilon}(a) = \frac{\varepsilon}{2}, P_{\varepsilon}(b) = 1 - \frac{\varepsilon}{2}$$

Then,

$$||P - Q||_1 = \varepsilon,$$

$$D_{KL}(P||Q) = \frac{\varepsilon}{2} \cdot \log \frac{\varepsilon}{2} = \infty.$$

3.2 A proof

Theorem 3.2. For two probability distributions P(x) and Q(x) that are defined over the same S, it holds that

$$D_{KL}(P||Q) \le \frac{1}{2\alpha_Q}||P - Q||_1^2,$$

where

$$\alpha_Q = \min_{x \in S} Q(x).$$

4 Misc

4.1 Total variation distance vs L_1 norm

Theorem 4.1. Scheffé's lemma.

For two probability distributions P(x) and Q(x) that are defined over the same S, it holds that

$$\delta(P,Q) = \frac{1}{2} ||P - Q||_1.$$

Proof. Let's refresh the definition of the total variation distance:

$$\delta(P,Q) = \max_{A \in 2^S} |P(A) - Q(A)|.$$
(5)

Denote by $G = \{x \in S \mid P(x) \ge Q(x)\}$. Try to find $A \subset S$ such that P(A) - Q(A) is maximized. Intuitively, it is the case when A = G.

Now, try to find $A' \subset S$ such that Q(A) - P(A) is maximized. Intuitively, it is the case when $A' = S \setminus G$.

Therefore, the subset A in $\delta(P,Q) = \max_{A \in 2^S} |P(A) - Q(A)|$ is either A = G or $A' = S \setminus G$. We will show that the maximum is obtained at both A and A':

$$P(G) - Q(G) = (1 - P(S \setminus G)) - (1 - Q(S \setminus G)) = Q(S \setminus G) - P(S \setminus G)$$

So if A maximizes P(X) - Q(X), A' maximizes Q(X) - P(X) and if A' maximizes P(X) - Q(X), then A maximizes Q(X) - P(X).

Now,

$$\begin{split} ||P - Q||_1 &= \sum_{x \in S} |P(x) - Q(x)| \\ &= \sum_{x \in G} (P(x) - Q(x)) + \sum_{x \in S \setminus G} (Q(x) - P(x)) \\ &= \delta(P, Q) + \delta(P, Q) \\ &= 2 \cdot \delta(P, Q) \end{split}$$

Let P and Q be probability distributions on the finite set A. Let $A_+ = \{a : Q(a) > 0\}$ and let $\alpha_Q = \min_{a \in A_+} Q(a)$.

How to prove that if $D(P||Q) < \infty$ then

$$D(P||Q) \leq rac{d^2(P,Q)}{lpha_q \cdot \ln 2},$$

where d(P,Q) is the variational distance of distributions P and Q, i.e., $d(P,Q) = \sum_{a \in A} |P(a) - Q(a)|.$

I was given a hint that first should prove that:

$$D(P||Q) \leq \sum_{a \in A_+} rac{P(a)}{\ln 2} (rac{P(a)}{Q(a)} - 1) = rac{1}{\ln 2} \sum_{a \in A_+} rac{|P(a) - Q(a)|^2}{Q(a)}.$$

statistics information-theory

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asked	Mar 1, 2020 at 15:25
	tefodos139 1

What did you try, and where are you stuck? Can you prove the hinted inequality? Can you conclude the argument assuming the hint? - stochasticboy321 Mar 5, 2020 at 4:07

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For the Hint from the right hand side to the middle is easy, hint distract the squared expression.

$$\begin{split} \sum_{a \in A_+} \frac{P(a)}{\ln 2} (\frac{P(a)}{Q(a)} - 1) &= \frac{1}{\ln 2} \sum_{a \in A_+} P(a) exp(ln \frac{P(a)}{Q(a)}) - 1 \geqslant \frac{1}{\ln 2} exp(\sum_{a \in A_+} P(a) ln(\frac{P(a)}{Q(a)})) - 1 \\ &\geqslant exp(D(P||Q)) - 1 \\ &\geqslant 1 + D(P||Q) - 1 = D(P||Q) \end{split}$$

For the reversed pinker's;

$$D(P||Q) \leqslant \frac{1}{\ln 2} \sum_{a \in A_+} \frac{|P(a) - Q(a)|^2}{Q(a)}$$
$$\leqslant \frac{1}{\ln 2} \sum_{a \in A_+} \frac{|P(a) - Q(a)|^2}{\min_{a \in A_+} Q(a)} \leqslant \frac{\max_{a \in A_+} |P(a) - Q(a)| \cdot \sum_{a \in A_+} |P(a) - Q(a)|}{\alpha_Q \cdot \ln 2} \leqslant \frac{d^2(P,Q)}{\alpha_Q \cdot \ln 2}$$

The last inequality you can deduce it after using scheffe's theorem for variational distance.