

1. Entropy, Cross-Entropy, Kullback - Leibler (KL)-divergence

- (a) Entropy is a measure of expected surprise. For a given discrete Random variable Y , we know that from Information Theory that a measure the surprise of observing that Y takes the value k by computing:

$$\log \frac{1}{p(Y = k)} = -\log[p(Y = k)]$$

As given:

- if $p(Y = k) \rightarrow 0$, the surprise of observing k approaches ∞
- if $p(Y = k) \rightarrow 1$, the surprise of observing k approaches 0

The Entropy of the distribution of Y is then the expected surprise given by:

$$H(Y) = E_Y \left[-\log(p(Y = k)) \right] = -\sum_k \left[p(Y = k) \log[p(Y = k)] \right]$$

On the other hand, Cross-entropy is a measure building upon entropy, generally calculating the difference between two probability distributions p and q . it is given by:

$$\begin{aligned} H(p, q) &= E_{p(x)} \left[\frac{1}{\log(q(x))} \right] \\ &= \sum_x \left[p(x) \log \left[\frac{1}{q(x)} \right] \right] \end{aligned}$$

Relative Entropy also known as KL Divergence measures how much one distribution diverges from another. For two discrete probability distributions, p and q , it is defined as:

$$D_{KL}(p||q) = \sum_x \left[p(x) \log \left[\frac{p(x)}{q(x)} \right] \right]$$

Let's define the following probability distributions given by:

$$\begin{aligned} p(x) &= \begin{cases} 1 & \text{with probability 0.5} \\ -1 & \text{with probability 0.5} \end{cases} \\ q(x) &= \begin{cases} 1 & \text{with probability 0.1} \\ -1 & \text{with probability 0.9} \end{cases} \end{aligned}$$

Show that KL-divergence is not symmetric and hence does not satisfy some intuitive attributes of distances.

- (b) Re-write $D_{KL}(p||q)$ in term of the Entropy $H(p)$ and the cross entropy $H(p, q)$.
- (c) Show that KL - divergence is always non-negative using Jensen's Inequality which states: $E[\log X] \leq \log E[X]$ and the fact that \log is a concave function.
- (d) Knowing that the equality in Jensen's inequality can only hold if X is a constant random variable, please state when is $D_{KL}(q||p) = 0$. ?

2. Simple Latent Variable Models

Formally, a latent variable model p is a probability distribution over observed variables x and latent variables z (variables that are not directly observed but inferred), $p_\theta(x, z)$. Because we know z is unobserved, using learning methods learned in class (like supervised learning methods) is unsuitable. Indeed, our learning problem of maximizing the log-likelihood of the data turns from:

$$\theta \leftarrow \arg \max_{\theta} \frac{1}{N} \sum_{i=1}^N \log[p_\theta(x_i)]$$

to:

$$\theta \leftarrow \arg \max_{\theta} \frac{1}{N} \sum_{i=1}^N \log\left[\int p_\theta(x_i | z)p(z)dz\right]$$

where $p(x)$ has become $\int p_\theta(x_i | z)p(z)dz$.

- (a) State whether or not we could directly maximize the likelihood above and why?
- (b) We define the proxy likelihood given by:

$$\mathcal{L}(x_i, \theta, \phi) = E_{z \sim q(z|x_i)} \left[\log[p_\theta(x_i | z)] \right] - D_{KL} \left[q(z | x_i) || p(z) \right]$$

Please show that $\mathcal{L}(x_i, \theta, \phi)$ is always a lower bound to the true log likelihood for x_i .

Hint: You can show that something is a lower bound by showing that adding a non-negative term to it gives the original quantity — remember, the KL divergence is always non-negative.

- (c) To optimize the Variational Lower Bound derived in the previous problem, which distribution do we sample z from?
- (d) To be able to take a derivative through a sampling operation, we need to show how sampling can be done as a deterministic and continuous function of functions of parameters as well as an external independent source of randomness. Otherwise, it is hard to understand how things would change a little bit if the parameters changed a little bit. Such explicit representations of sampling are called "the reparameterization trick" in machine-learning communities. Assume we have a normal distribution for x with both means and variance parameterized by parameters θ and we would like to solve for:

$$\min_{\theta} E_q[x^2]$$

Assuming that ϵ is an independent standard Normal $\mathcal{N}(0, 1)$ random variable, write x as a function of ϵ and use that to compute the gradient of the objective function above.

- (e) Describe step-by-step what happens during a forward pass during VAE training
- (f) Describe what the encoder and decoder of the VAE are doing to capture and encode this information into a latent representation of space z .
- (g) Once the VAE is trained, how do we use it to generate a new fresh sample from the learned approximation of the data-generating distribution.?

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