Understanding Variational Auto Encoder

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1. Understanding Variational Auto Encoder

Variational Auto Encoder (VAE)[1] encodes images into vectors in a latent space, and then decode the latent vectors into images. We denote

- z: latent variable, $z \in \mathbb{R}^J$
- x: data (images), $x \in \mathbb{R}^{H \cdot W}$
- p(x): evidence probability
- p(z): prior probability
- p(z|x): posterior probability
- p(x|z): likelihood probability

The goal is to find p(z|x) given p(z) and x. Once p(z|x) is known, for each sample in x, we can represent it with a low dimensional latent vector z by network forward propagration: $z \leftarrow p(z|x) \leftarrow x$. However,

$$p(z|x) = \frac{p(x|z)p(z)}{p(x)} = \frac{p(x|z)p(z)}{\int p(x|z)p(z)dz} = \frac{p(x|z)p(z)}{\int \int \int \int \int \int \dots p(x|z)p(z)dz}$$

p(z|x) is intractable due to the intractable denominator. We resort to variational inference which approximates p(z|x) with a distribution q(z|x) from a tractable family (e.g., Gaussian distribution). Then the task is translated to: find q(z|x) that is as close as possible to p(z|x). Formally, their distributional distance to be minimized is measured by KL divergence:

$$\begin{split} KL\left(q(z|x)||p(z|x)\right) &= -\int q(z|x)\log\frac{p(z|x)}{q(z|x)} \\ &= -\int q(z|x)\log\frac{p(x|z)p(z)/p(x)}{q(z|x)}\cdots using\ Bayesian\ theorem \\ &= -\int q(z|x)\log\frac{p(x|z)p(z)}{q(z|x)} + \int q(z|x)\log p(x) \\ &= -\int q(z|x)\log\frac{p(x|z)p(z)}{q(z|x)} + \log p(x)\int q(z|x)\cdots note\ that \int q(z|x) = 1 \\ &= \underbrace{-\int q(z|x)\log\frac{p(x|z)p(z)}{q(z|x)}}_{Evidence} + \underbrace{\log p(x)}_{Evidence} \\ &= \underbrace{-\int q(z|x)\log\frac{p(x|z)p(z)}{q(z|x)}}_{Evidence} + \underbrace{\log p(x)}_{Evidence} \end{split}$$

Since KL divergence is positive:

$$KL\left(q(z|x)\|p(z|x)\right) = \underbrace{-\int q(z|x)\log\frac{p(x|z)p(z)}{q(z|x)}}_{Evidence Lower Bound} + \underbrace{\log p(x)}_{Evidence} > 0$$

We derived what is called Evidence Lower Bound:

$$\underbrace{\log p(x)}_{Evidence} > \underbrace{\int q(z|x) \log \frac{p(x|z)p(z)}{q(z|x)}}_{Evidence Lower Bound}$$

More specifically:

$$\underbrace{\int q(z|x) \log \frac{p(x|z)p(z)}{q(z|x)}}_{EvidenceLowerBound} = \int q(z|x) \log \frac{p(z)}{q(z|x)} + \int q(z|x) \log \frac{p(x|z)}{q(z|x)}$$

$$= \underbrace{KL\left(q(z|x)\|p(z)\right)}_{Distribution} + \underbrace{\mathbb{E}_{q(z|x)} \log p(x|z)}_{Reconstruction}$$

Based on the above formulation, we finally arrive at the loss function:

$$\mathcal{L} = -\underbrace{KL\left(q(z|x)\|p(z)\right)}_{Distribution} - \underbrace{\mathbb{E}_{q(z|x)}\log p(x|z)}_{Reconstruction}$$

Minimizing the loss equals minimizing the distribution distance between q(z|x) and p(z|x). Most importantly, each item in \mathcal{L} is tractable:

- q(z|x): the encoder output $\{z_j \sim \mathcal{N}(\mu_j, \sigma_i^2) | j = 1, 2, \cdots, J\}$.
- p(z) is defined as Gaussian priors $\{z_j \sim \mathcal{N}(0,1) | j=1,2,\cdots,J\}$.
- $\log p(x|z) = \log \mathcal{N}(x \hat{\mu}, \hat{\sigma}^2)$

Calculating the loss[2]:

$$\mathcal{L} = -\underbrace{KL\left(q(z|x)||p(z)\right)}_{Distribution} - \underbrace{\mathbb{E}_{q(z|x)}\log p(x|z)}_{Reconstruction}$$

$$= \frac{1}{2} \sum_{j=1}^{J} \left(1 + \log\left((\sigma_j)^2\right) - (\mu_j)^2 - (\sigma_j)^2\right) - \sum_{m=1}^{H \cdot W} (x_m - \hat{\mu_m})^2$$

References

- [1] Diederik P Kingma and Max Welling. Auto-encoding variational bayes. arXiv preprint arXiv:1312.6114, 2013.
- [2] Stephen Odaibo. Tutorial: Deriving the standard variational autoencoder (vae) loss function. arXiv preprint arXiv:1907.08956, 2019.