Autoencoder and Variational Autoencoder

Zhe Chen, Dijing Zhang

K-Means Clustering

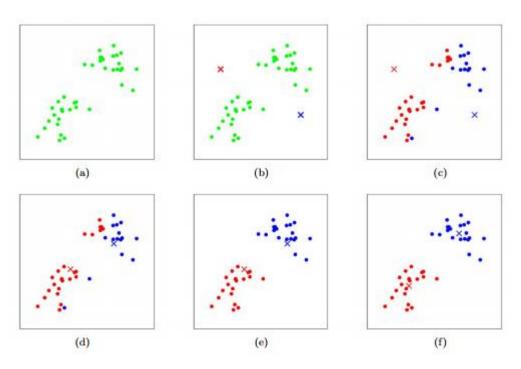


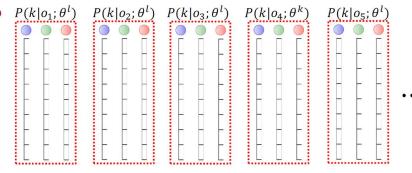
Figure 1: K-means algorithm. Training examples are shown as dots, and cluster centroids are shown as crosses. (a) Original dataset. (b) Random initial cluster centroids. (c-f) Illustration of running two iterations of k-means. In each iteration, we assign each training example to the closest cluster centroid (shown by "painting" the training examples the same color as the cluster centroid to which is assigned); then we move each cluster centroid to the mean of the points assigned to it. Images courtesy of Michael Jordan.

Reference: https://stanford.edu/~cpiech/cs221/handouts/kmeans.html

Expectation Maximization

EM for GMMs

In proportion to



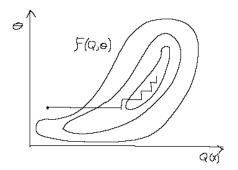
- Initialize μ_k^0 and Σ_k^0 for all k
- Iterate (over *l*):

- E: complete the data M: update estimates
- Compute $P(k|o;\theta^l)$ for all o
 - Compute the proportions by which o is assigned to all Gaussians
- Update:

$$- \mu_k^{l+1} = \frac{1}{\sum_o P(k|o;\theta^l)} \sum_o P(k|o;\theta^l) o$$

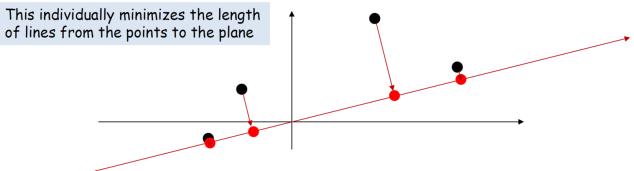
$$- \Sigma_k^{l+1} = \frac{1}{\sum_{o} P(k|o;\theta^l)} \sum_{o} P(k|o;\theta^l) (o - \mu_k^{l+1}) (o - \mu_k^{l+1})^T$$

Coordinate ascent

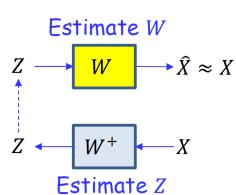


Reference: 10-701 EM Slides by Eric Xing

Linear Autoencoder = Iterative PCA



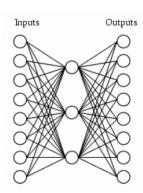
- Initialize a subspace (the basis w)
- Iterate until convergence:
 - Find the best position vectors Z on the W subspace for each training instance
 - Find the location on W that is *closest* to each instance, i.e. the perpendicular projection
 - Let W rotate and stretch/shrink, keeping the arrangement of Z locations fixed
 - Minimize the total square length of the lines attaching the projection on the place to the instance



Examples of Autoencoders

Binary Autoencoder

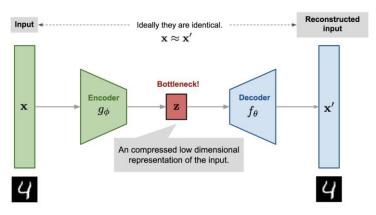
Network



Data/Target One-hot encodings of 0 to 7

Can we get the network to learn a binary latent vector?

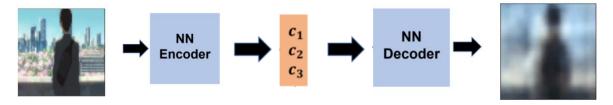
MNIST Autoencoder



MNIST dataset

How do we improve the quality of reconstructions?

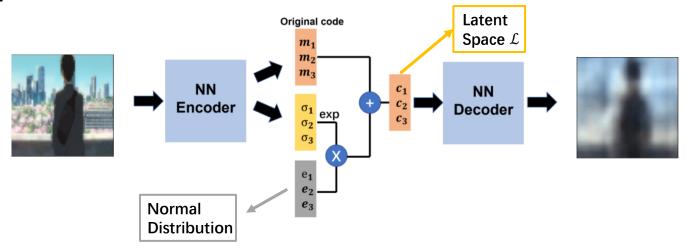
ΑE

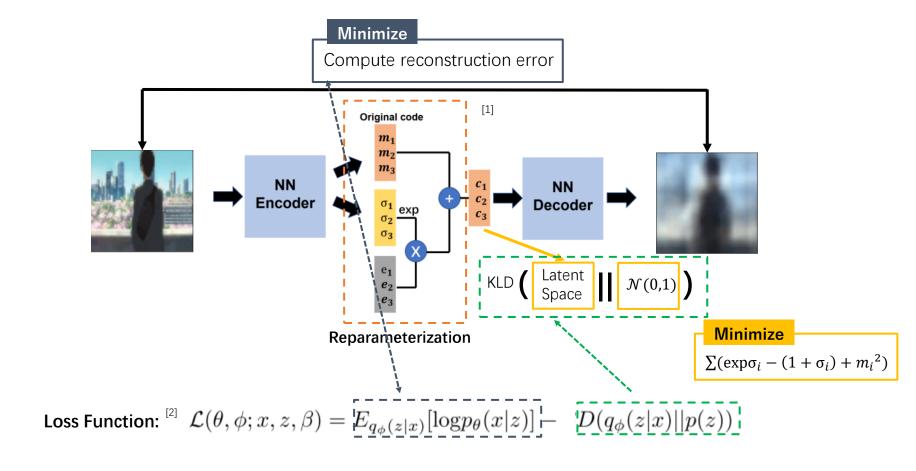


Can hardly learn a continuous latent space if we directly learn the code (ci) here.

But how about we introduce the distribution idea to the latent space, like making the space follow one distribution, so that it can be continuous?

VAE

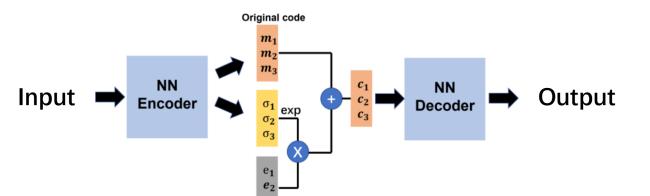




Reference:

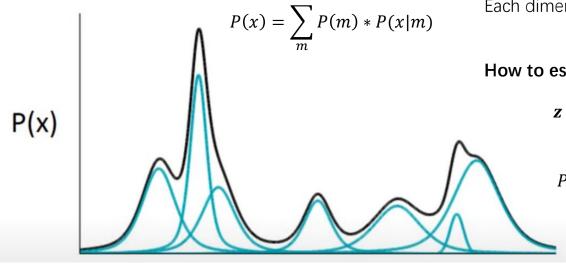
^[1] Hung-yi Lee's lecture https://www.youtube.com/watch?v=0CKeqXl5IY0&t=1650s

^[2] Higgins, Irina, et al. "beta-vae: Learning basic visual concepts with a constrained variational framework." (2016).



Hope to learn the probability distribution of output

Gaussian Mixture Model



 $z \sim N(0, I)$ z is a vector from normal distribution Each dimension of Z represents an attribute $x|z \sim N(\mu(z), \sigma(z))$

How to estimate $\mu(z)$, $\sigma(z)$?

$$z \implies NN \implies \mu(z), \sigma(z)$$

$$P(x) = \int_{z} P(z) * P(x|z) dz$$

$$P(x) = \int_{z} P(z) * P(x|z) dz$$

Tune the NN parameters to max likelihood of the observed x: $L = \sum_{x} log P(x)$

$$z \longrightarrow NN \longrightarrow \mu(z), \sigma(z)$$
Decoder

Another distribution q(z|x):

$$z|x\sim N(\mu'(x),\sigma'(x))$$

$$x \longrightarrow NN \longrightarrow \mu'(x), \sigma'(x)$$

Encoder

$$log P(x) = \int_{z} q(z|x)log P(x)dz \qquad s.t. \int_{z} q(z|x)dz = 1 \text{ and } q \text{ can be any distribution}$$

$$= \int_{z} q(z|x)log \frac{P(z,x)}{P(z|x)}dz = \int_{z} q(z|x)log(\frac{P(z,x)}{q(z|x)} * \frac{q(z|x)}{P(z|x)})dz$$

$$= \int_{z} q(z|x)log \frac{P(z,x)}{q(z|x)}dz + \int_{z} q(z|x)log \frac{q(z|x)}{P(z|x)}dz$$

$$= \int_{z} q(z|x)log \frac{P(z,x)}{q(z|x)}dz + \int_{z} q(z|x)log \frac{q(z|x)}{P(z|x)}dz$$

$$KLD(q(z|x))$$

$$*KLD(p||q) = \sum_{z} p * \log \frac{p}{q}$$
$$KLD(q(z|x)||P(z|x)) \ge 0$$

 $\geq \int q(z|x) \log \frac{P(z,x)}{q(z|x)} dz$ Evidence Lower Bound(ELBO) L_b

$$log P(x) = L_b + KLD(q(z|x)||P(z|x)) \sim N(0,||z|)$$

$$L_b = \int_{z} q(z|x) \log \frac{P(z,x)}{q(z|x)} dz = \int_{z} q(z|x) \log \frac{P(x|z) * P(z)}{q(z|x)} dz$$

Find q(z|x) and P(x|z) to $\max L_b$

$$= \int_{-\infty}^{\infty} q(z|x) \log \frac{P(z)}{q(z|x)} dz + \int_{-\infty}^{\infty} q(z|x) \log P(x|z) dz$$

$$= -KLD\left(q(z|x)\right)|P(z) + \int_{z} q(z|x) \log P(x|z) dz$$

$$z|x \sim N(\mu'(x), \sigma'(x))$$

1. Minimize
$$KLD(q(z|x)||P(z))$$
:

$\frac{\text{Minimize}}{\sum (\exp \sigma_i - (1 + \sigma_i) + m_i^2)}$

 $x \longrightarrow NN \longrightarrow \mu'(x), \sigma'(x)$

Encoder

2. Maximize $\int_{z} q(z|x) \log P(x|z) dz$ $= E_{q(z|x)}[\log P(x|z)]$ Minimize

Compute reconstruction error

$$\Rightarrow \frac{\mu'(x)}{\sigma'(x)} \Rightarrow z \Longrightarrow$$



 $\downarrow \mu(x) \stackrel{\text{close}}{\longleftarrow} \\
\sigma(x)$