Variational Autoencoders

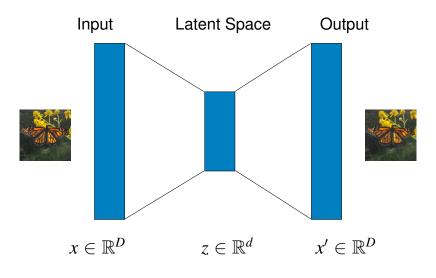
Geometry of Data

October 22, 2020

Talking about this paper:

Diederik Kingma and Max Welling, Auto-Encoding Variational Bayes, In *International Conference on Learning Representation (ICLR)*, 2014.

Autoencoders

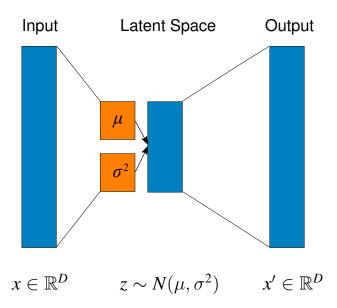


$$d \ll D$$

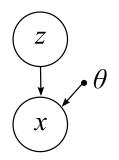
Autoencoders

- Linear activation functions give you PCA
- Training:
 - 1. Given data x, feedforward to x' output
 - 2. Compute loss, e.g., $L(x, x') = ||x x'||^2$
 - 3. Backpropagate loss gradient to update weights
- Not a generative model!

Variational Autoencoders



Generative Models



Sample a new x in two steps:

Prior: p(z)Generator: $p_{\theta}(x \mid z)$

Now the analogy to the "encoder" is:

Posterior: $p(z \mid x)$

Bayesian Inference

Posterior via Bayes' Rule:

$$p(z \mid x) = \frac{p_{\theta}(x \mid z)p(z)}{p(x)}$$
$$= \frac{p_{\theta}(x \mid z)p(z)}{\int p_{\theta}(x \mid z)p(z)dz}$$

Integral in denominator is (usually) intractable!

Could use Monte Carlo to approximate, but it's expensive

Kullback-Leibler Divergence

$$D_{ ext{KL}}(q||p) = -\int q(z) \log \left(rac{p(z)}{q(z)}
ight) dz$$
 $= E_q \left[-\log \left(rac{p}{q}
ight)
ight]$

The average information gained from moving from q to p

Variational Inference

Approximate intractable posterior $p(z \mid x)$ with a manageable distribution q(z)

Minimize the KL divergence: $D_{\text{KL}}(q(z)||p(z \mid x))$

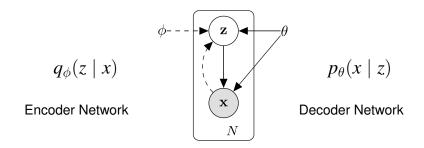
Evidence Lower Bound (ELBO)

$$\begin{aligned} D_{\text{KL}}(q(z) || p(z | x)) \\ &= E_q \left[-\log \left(\frac{p(z | x)}{q(z)} \right) \right] \\ &= E_q \left[-\log \frac{p(z, x)}{q(z)p(x)} \right] \\ &= E_q [-\log p(z, x) + \log q(z) + \log p(x)] \\ &= -E_q [\log p(z, x)] + E_q [\log q(z)] + \log p(x) \end{aligned}$$

$$\log p(x) = D_{\mathrm{KL}}(q(z) \| p(z \mid x)) + L[q(z)]$$

ELBO: $L[q(z)] = E_q[\log p(z,x)] - E_q[\log q(z)]$

Variational Autoencoder



Maximize ELBO:

$$\mathcal{L}(\theta, \phi, x) = E_{q_{\phi}}[\log p_{\theta}(x, z) - \log q_{\phi}(z \mid x)]$$

VAE ELBO

$$\begin{split} \mathcal{L}(\theta, \phi, x) &= E_{q_{\phi}}[\log p_{\theta}(x, z) - \log q_{\phi}(z \mid x)] \\ &= E_{q_{\phi}}[\log p_{\theta}(z) + \log p_{\theta}(x \mid z) - \log q_{\phi}(z \mid x)] \\ &= E_{q_{\phi}}\left[\log \frac{p_{\theta}(z)}{q_{\phi}(z \mid x)} + \log p_{\theta}(x \mid z)\right] \\ &= -D_{\text{KL}}(q_{\phi}(z \mid x) || p_{\theta}(z)) + E_{q_{\phi}}[\log p_{\theta}(x \mid z)] \end{split}$$

Problem: Gradient $\nabla_{\phi} E_{q_{\phi}}[\log p_{\theta}(x \mid z)]$ is intractable! Use Monte Carlo approx., sampling $z^{(s)} \sim q_{\phi}(z \mid x)$:

$$\nabla_{\phi} E_{q_{\phi}}[\log p_{\theta}(x \mid z)] \approx \frac{1}{S} \sum_{i=1}^{S} \log p_{\theta}(x \mid z) \nabla_{\phi} \log q_{\phi}(z^{(s)} \mid x)$$

Reparameterization Trick

What about the other term?

$$-D_{\mathrm{KL}}(q_{\phi}(z\mid x)||p_{\theta}(z))$$

Says encoder, $q_{\phi}(z\mid x)$, should make code z look like prior distribution

Instead of encoding z, encode parameters for a normal distribution, $N(\mu,\sigma^2)$

Reparameterization Trick

$$q_{\phi}(z_j \mid x^{(i)}) = N(\mu_j^{(i)}, \sigma_j^{2(i)})$$

 $p_{\theta}(z) = N(0, I)$

KL divergence between these two is:

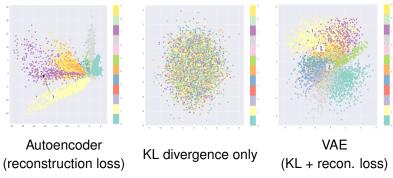
$$D_{\mathrm{KL}}(q_{\phi}(z \mid x^{(i)}) || p_{\theta}(z)) = -\frac{1}{2} \sum_{i=1}^{d} \left(1 + \log(\sigma_{j}^{2(i)}) - (\mu_{j}^{(i)})^{2} - \sigma_{j}^{2(i)} \right)$$

Results from Kingma & Welling

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Why Do Variational?

Example trained on MNIST:



From: this webpage