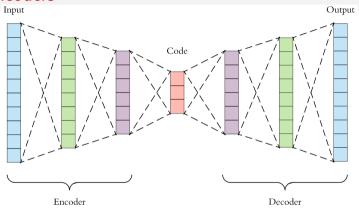
### Vineeth N Balasubramanian

Department of Computer Science and Engineering Indian Institute of Technology, Hyderabad



## Recall: Autoencoders

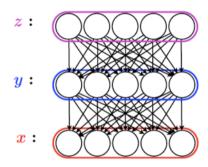


Autoencoders can reconstruct data, and can learn features to initialize a supervised model.

Can we generate images from an autoencoder?

Credit: Arden Dertat, TowardsDataScience

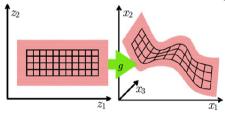
- Introduced around the same time by two groups of researchers:
  - Kingma and Welling, Auto-Encoding Variational Bayes, ICLR 2014
  - Rezende, Mohamed and Wiestra,
     Stochastic Backpropagation and
     Variational Inference in Deep Latent
     Gaussian Models, ICML 2014



• Latent Variable Model: Learn a mapping from some latent variable z to a possibly complex distribution on x

$$p(x) = \int p(x,z)dz$$
 where  $p(x,z) = p(x|z)p(z)$   
 $p(z) = \text{something simple};$   $p(x|z) = g(z)$ 

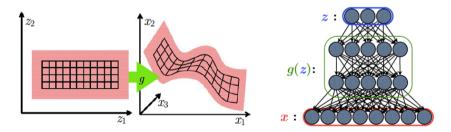
 Can we learn to decouple the true explanatory factors (latent variables) underlying the data distribution (e.g. identity and expression in face images)? How?



Credit: Aaron Courville, Deep Learning Summer School, 2015

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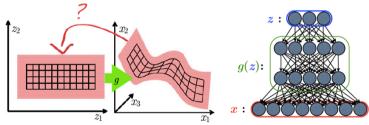
• Leverage neural networks to learn a latent variable model! 
$$p(x)=\int p(x,z)dz \quad \text{where} \quad p(x,z)=p(x|z)p(z)$$
 
$$p(z)=\text{something simple;} \quad p(x|z)=g(z)$$



• Leverage neural networks to learn a latent variable model!

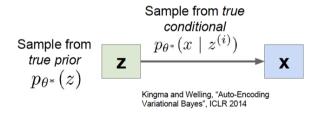
$$p(x) = \int p(x, z)dz$$
 where  $p(x, z) = p(x|z)p(z)$   
 $p(z) = \text{something simple};$   $p(x|z) = g(z)$ 

• Where does z come from? Computing the posterior p(z|x) is intractable, and we need it to train the directed model



A Bayesian spin on an autoencoder!

Assume our data  $\{x^{(i)}\}_{i=1}^{N}$  is generated like this:



Credit: Fei-Fei Li, Andrej Karpathy and Justin Johnson, CS231n, Stanford Univ

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A Bayesian spin on an autoencoder!

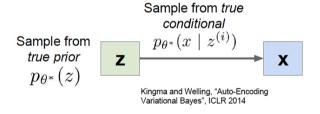
Assume our data  $\{x^{(i)}\}_{i=1}^{N}$  is generated like this:

Sample from true conditional Sample from true  $p_{\theta^*}(x \mid z^{(i)})$   $\mathbf{x}$  Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

• **Intuition:** x is an image, z gives class, orientation, attributes, etc

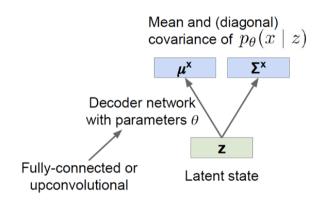
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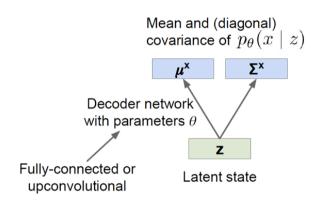


• **Intuition:** x is an image, z gives class, orientation, attributes, etc

• **Problem:** Estimate  $\theta$  without access to latent states  $z^{(i)}$ 

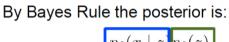


• **Prior:** Assume  $p_{\theta}(z)$  is a unit Gaussian



• **Prior:** Assume  $p_{\theta}(z)$  is a unit Gaussian

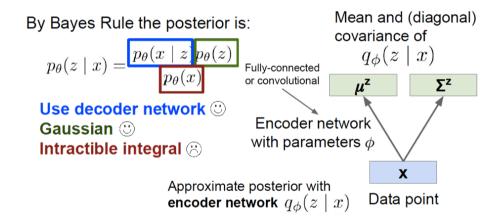
• Conditional: Assume  $p_{\theta}(x|z)$  is a diagonal Gaussian, predict mean and variance with neural network

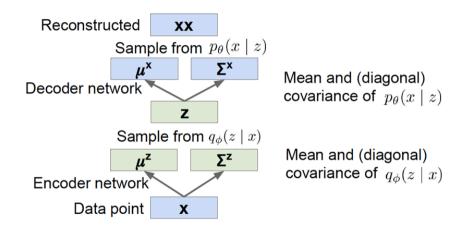


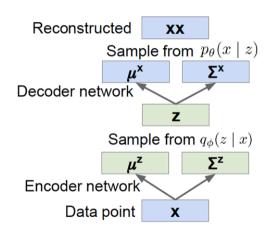
$$p_{\theta}(z \mid x) = \frac{p_{\theta}(x \mid z) p_{\theta}(z)}{p_{\theta}(x)}$$

Use decoder network ①
Gaussian ②
Intractible integral ②

Mean and (diagonal) covariance of Encoder network with parameters  $\phi$ X Data point







Training like a normal autoencoder: reconstruction loss at the end, regularization toward prior in middle Mean and (diagonal) covariance of  $p_{\theta}(x \mid z)$ 

Mean and (diagonal) covariance of  $q_{\phi}(z \mid x)$  (should be close to prior  $p_{\theta}(z)$ )

(should be close to data x)

$$\theta^* = \arg\max_{\theta} \prod_{i=1}^N p_{\theta}(x^{(i)})$$
 Maximize likelihood of dataset  $\{x^{(i)}\}_{i=1}^N$ 

$$\begin{split} \theta^* &= \arg\max_{\theta} \prod_{i=1}^N p_{\theta}(x^{(i)}) & \text{Maximize likelihood of dataset } \left\{x^{(i)}\right\}_{i=1}^N \\ &= \arg\max_{\theta} \sum_{i=1}^N \log p_{\theta}(x^{(i)}) & \text{Maximize log-likelihood instead because sums are nicer} \end{split}$$

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$$p_{\theta}(x^{(i)}) = \int p_{\theta}(x^{(i)}, z) dz$$
 Marginalize joint distribution

$$\theta^* = \arg\max_{\theta} \prod_{i=1}^N p_{\theta}(x^{(i)}) \qquad \text{Maximize likelihood of dataset } \left\{x^{(i)}\right\}_{i=1}^N$$
 
$$= \arg\max_{\theta} \sum_{i=1}^N \log p_{\theta}(x^{(i)}) \qquad \text{Maximize log-likelihood instead because sums are nicer}$$
 
$$p_{\theta}(x^{(i)}) = \int p_{\theta}(x^{(i)}, z) dz \qquad \text{Marginalize joint distribution}$$
 
$$= \int p_{\theta}(x^{(i)} \mid z) p_{\theta}(z) dz \qquad \text{Intractible integral} \ \odot$$

$$\begin{split} \log p_{\theta}(x^{(i)}) &= \mathbf{E}_{z \sim q_{\phi}(z|x^{(i)})} \left[ \log p_{\theta}(x^{(i)}) \right] \quad (p_{\theta}(x^{(i)}) \text{ Does not depend on } z) \\ &= \mathbf{E}_{z} \left[ \log \frac{p_{\theta}(x^{(i)} \mid z) p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})} \right] \quad \text{(Bayes' Rule)} \\ &= \mathbf{E}_{z} \left[ \log \frac{p_{\theta}(x^{(i)} \mid z) p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})} \frac{q_{\phi}(z \mid x^{(i)})}{q_{\phi}(z \mid x^{(i)})} \right] \quad \text{(Multiply by constant)} \end{split}$$

Credit: Fei-Fei Li, Andrej Karpathy and Justin Johnson, CS231n, Stanford Univ

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$$\begin{split} \log p_{\theta}(x^{(i)}) &= \mathbf{E}_{z \sim q_{\phi}(z|x^{(i)})} \left[ \log p_{\theta}(x^{(i)}) \right] \quad (p_{\theta}(x^{(i)}) \text{ Does not depend on } z) \\ &= \mathbf{E}_{z} \left[ \log \frac{p_{\theta}(x^{(i)} \mid z) p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})} \right] \quad \text{(Bayes' Rule)} \\ &= \mathbf{E}_{z} \left[ \log \frac{p_{\theta}(x^{(i)} \mid z) p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})} \frac{q_{\phi}(z \mid x^{(i)})}{q_{\phi}(z \mid x^{(i)})} \right] \quad \text{(Multiply by constant)} \\ &= \mathbf{E}_{z} \left[ \log p_{\theta}(x^{(i)} \mid z) \right] - \mathbf{E}_{z} \left[ \log \frac{q_{\phi}(z \mid x^{(i)})}{p_{\theta}(z)} \right] + \mathbf{E}_{z} \left[ \log \frac{q_{\phi}(z \mid x^{(i)})}{p_{\theta}(z \mid x^{(i)})} \right] \quad \text{(Logarithms)} \\ &= \underbrace{\mathbf{E}_{z} \left[ \log p_{\theta}(x^{(i)} \mid z) \right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) || p_{\theta}(z))}_{\mathcal{D}(x^{(i)}, \theta, \phi)} \quad \text{``Elbow''} \\ &\geq 0 \end{split}$$

Credit: Fei-Fei Li, Andrej Karpathy and Justin Johnson, CS231n, Stanford Univ

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$$\begin{split} \log p_{\theta}(x^{(i)}) &= \mathbf{E}_{z \sim q_{\phi}(z|x^{(i)})} \left[ \log p_{\theta}(x^{(i)}) \right] \quad (p_{\theta}(x^{(i)}) \text{ Does not depend on } z) \\ &= \mathbf{E}_{z} \left[ \log \frac{p_{\theta}(x^{(i)} \mid z) p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})} \right] \quad \text{(Bayes' Rule)} \\ &= \mathbf{E}_{z} \left[ \log \frac{p_{\theta}(x^{(i)} \mid z) p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})} \frac{q_{\phi}(z \mid x^{(i)})}{q_{\phi}(z \mid x^{(i)})} \right] \quad \text{(Multiply by constant)} \\ &= \mathbf{E}_{z} \left[ \log p_{\theta}(x^{(i)} \mid z) \right] - \mathbf{E}_{z} \left[ \log \frac{q_{\phi}(z \mid x^{(i)})}{p_{\theta}(z)} \right] + \mathbf{E}_{z} \left[ \log \frac{q_{\phi}(z \mid x^{(i)})}{p_{\theta}(z \mid x^{(i)})} \right] \quad \text{(Logarithms)} \\ &= \underbrace{\mathbf{E}_{z} \left[ \log p_{\theta}(x^{(i)} \mid z) \right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) || p_{\theta}(z))}_{\mathcal{D}(x^{(i)}, \theta, \phi)} + \underbrace{D_{KL}(q_{\phi}(z \mid x^{(i)}) || p_{\theta}(z \mid x^{(i)}))}_{\geq 0} \right]}_{\mathcal{D}(x^{(i)}, \theta, \phi)} \\ &= \underbrace{\log p_{\theta}(x^{(i)} \mid z) \right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) || p_{\theta}(z \mid x^{(i)}))}_{\geq 0} \\ &= \underbrace{\log p_{\theta}(x^{(i)} \mid z) \right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) || p_{\theta}(z \mid x^{(i)}))}_{\geq 0} \\ &= \underbrace{\log p_{\theta}(x^{(i)} \mid z) \right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) || p_{\theta}(z \mid x^{(i)}))}_{\geq 0} \\ &= \underbrace{\log p_{\theta}(x^{(i)} \mid z) \right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) || p_{\theta}(z \mid x^{(i)}))}_{\geq 0} \\ &= \underbrace{\log p_{\theta}(x^{(i)} \mid z) \right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) || p_{\theta}(z \mid x^{(i)}))}_{\geq 0} \\ &= \underbrace{\log p_{\theta}(x^{(i)} \mid z) \right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) || p_{\theta}(z \mid x^{(i)}))}_{\geq 0} \\ &= \underbrace{\log p_{\theta}(x^{(i)} \mid z) \right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) || p_{\theta}(z \mid x^{(i)})}_{\geq 0} \\ &= \underbrace{\log p_{\theta}(x^{(i)} \mid z) \right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) || p_{\theta}(z \mid x^{(i)})}_{\geq 0} \\ &= \underbrace{\log p_{\theta}(x^{(i)} \mid z) \right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) || p_{\theta}(z \mid x^{(i)})}_{\geq 0} \\ &= \underbrace{\log p_{\theta}(x^{(i)} \mid z) \right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) || p_{\theta}(z \mid x^{(i)})}_{\geq 0} \\ &= \underbrace{\log p_{\theta}(x^{(i)} \mid z) \right] - \underbrace{\log p_{\theta}(x^{(i)} \mid z)}_{\geq 0} \\ &= \underbrace{\log p_{\theta}(x^{(i)} \mid z) \right] - \underbrace{\log p_{\theta}(x^{(i)} \mid z)}_{\geq 0} \\ &= \underbrace{\log p_{\theta}(x^{(i)} \mid z) \right] - \underbrace{\log p_{\theta}(x^{(i)} \mid z)}_{\geq 0} \\ &= \underbrace{\log p_{\theta}(x^{(i)} \mid z) \right] - \underbrace{\log p_{\theta}(x^{(i)} \mid z)}_{\geq 0} \\ &= \underbrace{\log p_{\theta}(x^{(i)} \mid z) \right] - \underbrace{\log p_{\theta}(x^{(i)} \mid z)}_{\geq 0} \\ &= \underbrace{\log p_{\theta}(x^{(i)} \mid z) \right] - \underbrace{\log p_{\theta}(x^{(i)} \mid z)}_{\geq 0} \\ &= \underbrace{\log p_{\theta}(x^{(i)} \mid z) \right] - \underbrace{\log p_{\theta}(x^{(i)} \mid z)}_{\geq 0}$$

Credit: Fei-Fei Li, Andrej Karpathy and Justin Johnson, CS231n, Stanford Univ

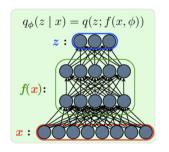
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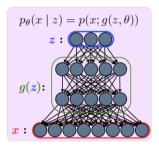
## Variational Autoencoder: Inference

• Introduce an inference model  $q_{\phi}(z|x)$  that learns to approximates the intractable posterior  $p_{\theta}(z|x)$  by optimizing the variational lower bound:

$$\mathcal{L}(\theta, \phi, x) = -D_{KL}(q_{\phi}(z|x)||p_{\theta}(z)) + \mathbb{E}_{q_{\phi}(z|x)}[\log p_{\theta}(x|z)]$$

• We parametrize  $q_{\phi}(z|x)$  with another neural network:





## Variational Autoencoder: How to train?

$$\mathcal{L}_{VAE} = \mathbb{E}_{q_{\phi}(z|x)} \left[ \log \frac{p_{\theta}(z,x)}{q_{\phi}(z|x)} \right]$$
$$= -D_{KL}(q_{\phi}(z|x)||p_{\theta}(z)) + \mathbb{E}_{q_{\phi}(z|x)}[\log p_{\theta}(x|z)]$$

•  $z \sim q_{\phi}(z|x)$ : need to differentiate through the sampling process; how to update  $\phi$ ? (encoder is probabilistic)

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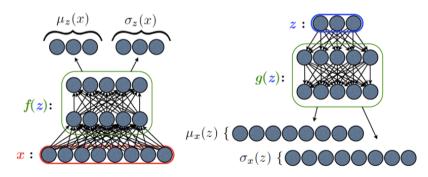
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- $z \sim q_{\phi}(z|x)$ : need to differentiate through the sampling process; how to update  $\phi$ ? (encoder is probabilistic)
- Solution: Make the randomness independent of encoder output, thus making the encoder deterministic; how?

# Reparametrization Trick

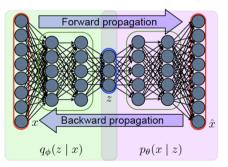
- Let's consider z to be real and  $q_{\phi}(z|x) = \mathcal{N}(z; u_z(x), \sigma_z(x))$
- Parametrize z as  $z = \mu_z(z) + \sigma_z(x)\epsilon_z$  where  $\epsilon_z = \mathcal{N}(0,1)$



# Training with Backpropagation

With the reparametrization trick, we can simultaneously train both the generative model  $p_{\theta}(x|z)$  and the inference model  $q_{\phi}(z|x)$  using backpropagation

Objective function:  $\mathcal{L}(\theta, \phi, x) = -D_{KL}(q_{\phi}(z|x)||p_{\theta}(z)) + \mathbb{E}_{q_{\phi}(z|x)}[\log p_{\theta}(x|z)]$ 



# VAE: Summary

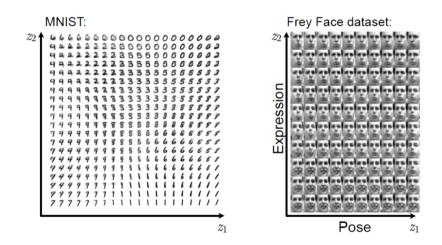
#### Traditional Autoencoders

- Learned by reconstructing input
- Used to learn features, initialize supervised models (not much anymore though)

#### Variational Autoencoders

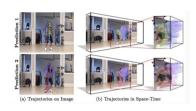
- Bayesian learning meets deep learning
- Sample from model to generate images

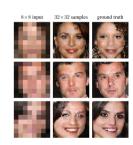
# VAE: What can they do?



# Applications of VAEs

- Image and video generation
- Superresolution
- Forecasting from static images
- Image inpainting
- many more...





Credit: Dahl et al, Pixel Recursive Super Resolution, ICCV 2017

## A Few Variants and Extensions

- Semi-Supervised VAEs
  - Kingma et al, Semi-Supervised Learning with Deep Generative Models, NeurIPS 2014
- Conditional VAE
  - Sohn et al, Learning Structured Output Representation using Deep Conditional Generative Models, NeurIPS 2015
- Importance-Weighted VAE
  - Burda et al, Importance Weighted Autoencoders, ICLR 2016
- Denoising VAE
  - Jiwoong et al, Denoising Criterion for Variational Auto-encoding Framework, AAAI 2017
- Inverse Graphics Network
  - Kulkarni et al, Deep Convolutional Inverse Graphics Network, NeurIPS 2015
- Adversarial Autoencoders
  - Makhzani et al, Adversarial Autoencoders, ICLR 2016

### Homework

### Readings

- Carl Doersch, Tutorial on Variational Autoencoder, arXiv 2016
- VAE example in PyTorch
- Kingma and Welling, Auto-Encoding Variational Bayes, ICLR 2014

#### Question

- Why does the encoder of a VAE map to a vector of means and a vector of standard deviations? Why does it not instead map to a vector of means and a covariance matrix?
- What about the decoder? If we assume a Mean Squared Error for the reconstruction loss, what is the covariance of the p(x|z) Gaussian distribution?