Variational Autoencoders

Probabilistic spin on autoencoders - will let us sample from the model to generate data!

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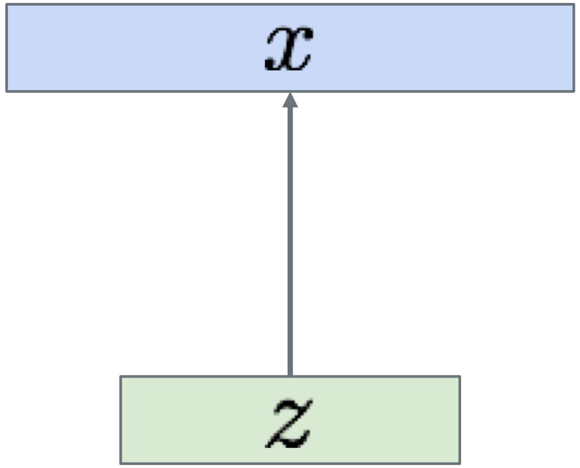
Assume training data $\{x^{(i)}\}_{i=1}^{N}$ enerated from underlying unobserved (latent) representation **z**

Sample from
true conditional
$p_{\theta^*}(x \mid z^{(i)})$



Sample from
true prior
$p_{\theta^*}(z)$

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders

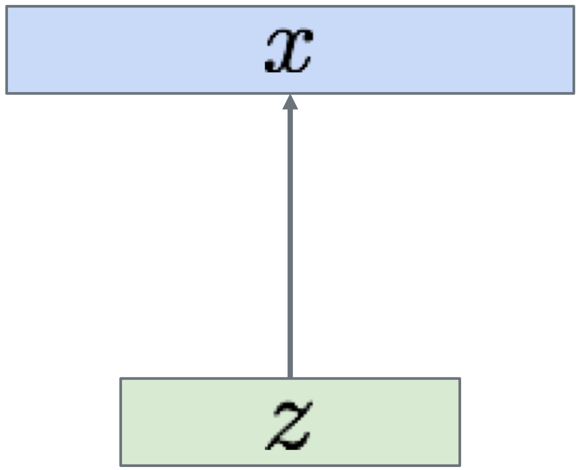
Probabilistic spin on autoencoders - will let us sample from the model to generate data!

Assume training data $\{x^{(i)}\}_{i=1}^{N}$ enerated from underlying unobserved (latent) representation **z**

Intuition (remember from autoencoders!): **x** is an image, **z** is latent factors used to generate **x:** attributes, orientation, etc.

Sample from true conditional

$p_{\theta^*}(x \mid z^{(i)})$



Sample from true prior

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Variational Autoencoders

We want to estimate the true parameters θ^* of this generative model.

Sample from true conditional

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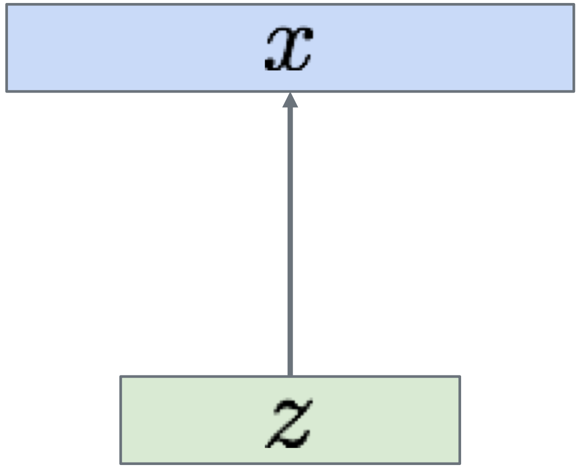

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Variational Autoencoders

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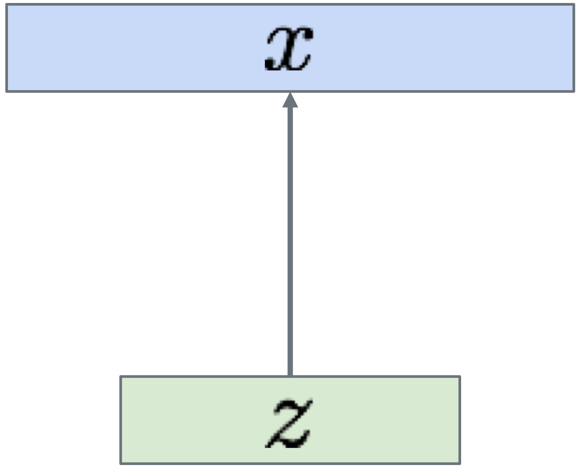

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How should we represent this model?

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Variational Autoencoders

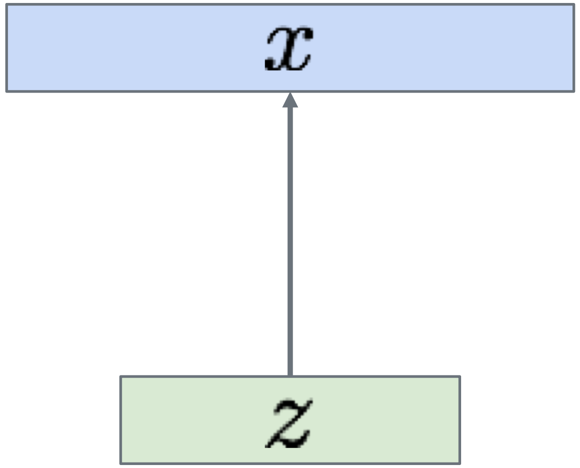
We want to estimate the true parameters θ^* of this generative model.

How should we represent this model?

Choose prior p(z) to be simple, e.g. Gaussian. Reasonable for latent attributes, e.g. pose, how much smile.

Sample from true conditional

$p_{\theta^*}(x \mid z^{(i)})$



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Variational Autoencoders

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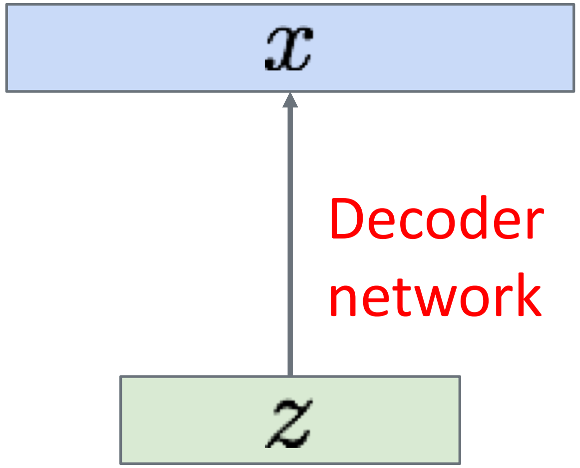

We want to estimate the true parameters θ^* of this generative model.

How should we represent this model?

Choose prior p(z) to be simple, e.g. Gaussian.

Conditional p(x|z) is complex (generates image)
=> represent with neural network

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Variational Autoencoders

We want to estimate the true parameters θ^* of this generative model.

How to train the model?

Sample from true conditional
$p_{\theta^*}(x \mid z^{(i)})$

Sample from true prior
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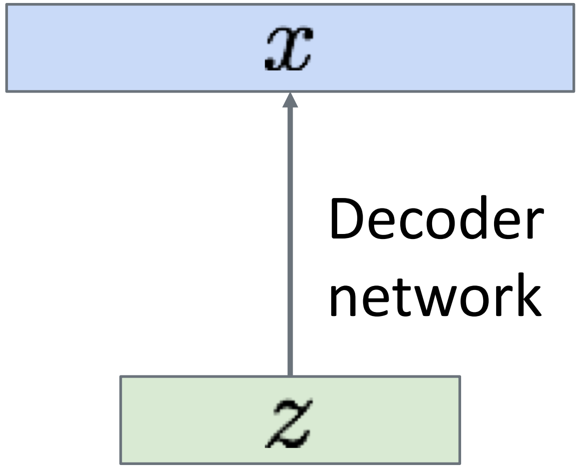

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Variational Autoencoders

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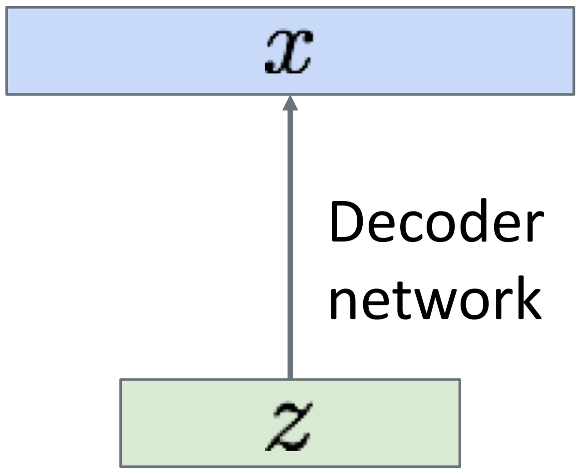

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How to train the model?

Remember strategy for training generative models from FVBNs. Learn model parameters to maximize likelihood of training data

$$p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$$

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders

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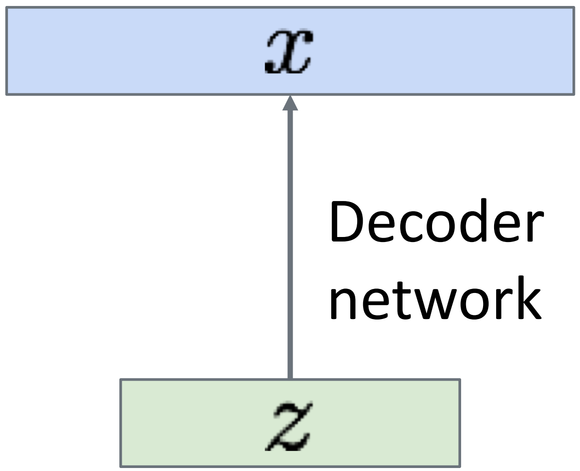

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Now with latent z

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Slide credit: Fei-Fei Li, Justin Johnson, Serena Yeung

Variational Autoencoders

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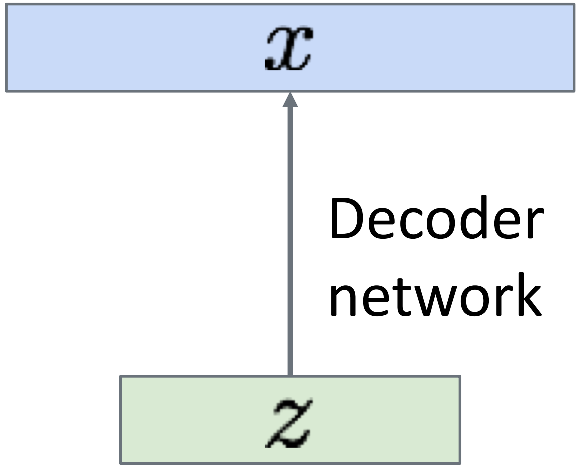

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Q: What is the problem with this?

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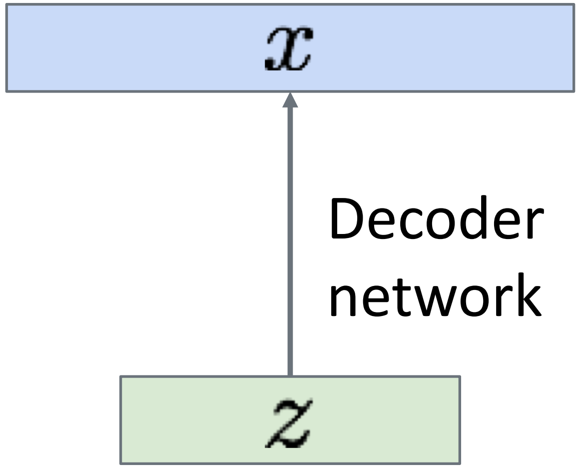

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Intractable!

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders: Intractability

Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders: Intractability

Data likelihood: $p_\theta(x) = \int p_\theta(z)p_\theta(x|z)dz$

Simple Gaussian prior

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders: Intractability

Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$

Decoder neural network

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Slide credit: Fei-Fei Li, Justin Johnson, Serena Yeung

Variational Autoencoders: Intractability

😢

Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$

Intractible to compute
p(x|z) for every z!

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders: Intractability

😢

Data likelihood: $p_\theta(x) = \int p_\theta(z)p_\theta(x|z)dz$

Intuitively, need to figure out which z corresponds to each x in the dataset, but such mapping is unknown.

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders: Intractability

Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$ 😢

Intuitively, need to figure out which z corresponds to each x in the dataset, but such mapping is unknown.

$$p_\theta(z|x) = p_\theta(x|z) p_\theta(z) / p_\theta(x)$$

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders: Intractability

Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$

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Posterior density also intractable: $p_\theta(z|x) = p_\theta(x|z) p_\theta(z) / p_\theta(x)$

Intractable data likelihood

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

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Variational Autoencoders: Intractability

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Posterior density also intractable: $p_\theta(z|x) = p_\theta(x|z)p_\theta(z)/p_\theta(x)$

Intractable data likelihood

Solution: In addition to decoder network modeling $p_\theta(x|z)$, define additional encoder network $q_\phi(z|x)$ that approximates $p_\theta(z|x)$

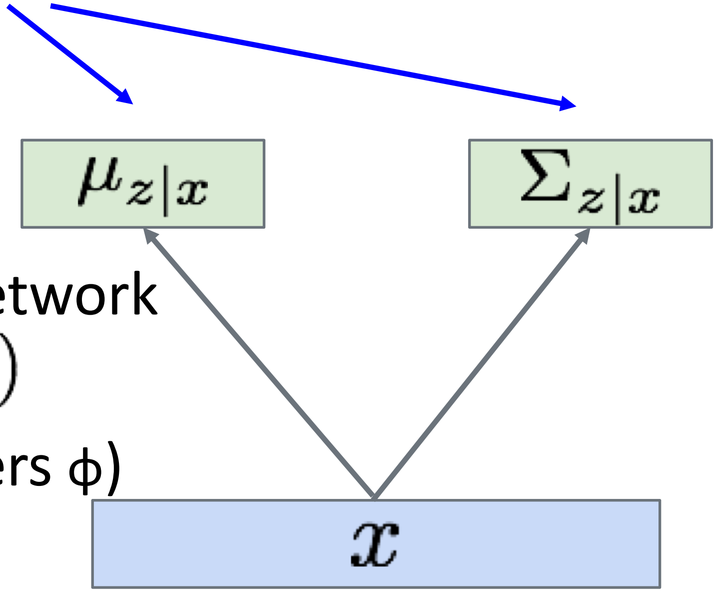
Will see that this allows us to derive a lower bound on the data likelihood that is tractable, which we can optimize

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders

Since we're modeling probabilistic generation of data, encoder and decoder networks are probabilistic

Mean and (diagonal) covariance of **z | x**

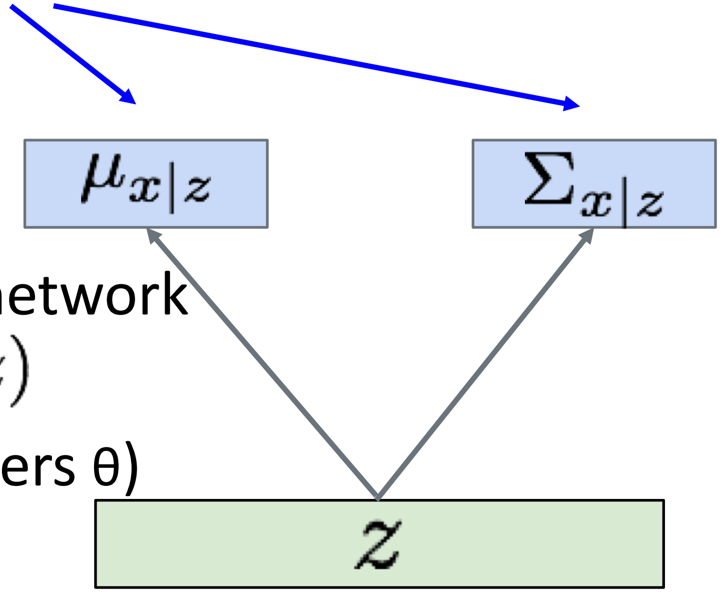


Encoder network

$q_\phi(z|x)$

(parameters ϕ)

Mean and (diagonal) covariance of **x | z**



Decoder network

$p_\theta(x|z)$

(parameters θ)

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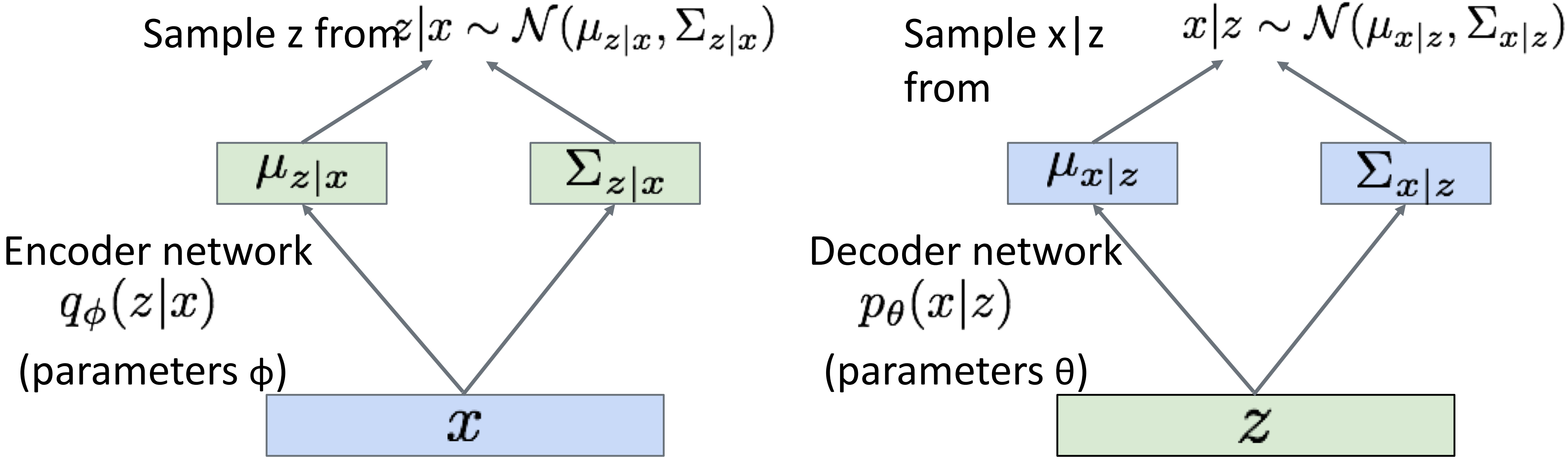

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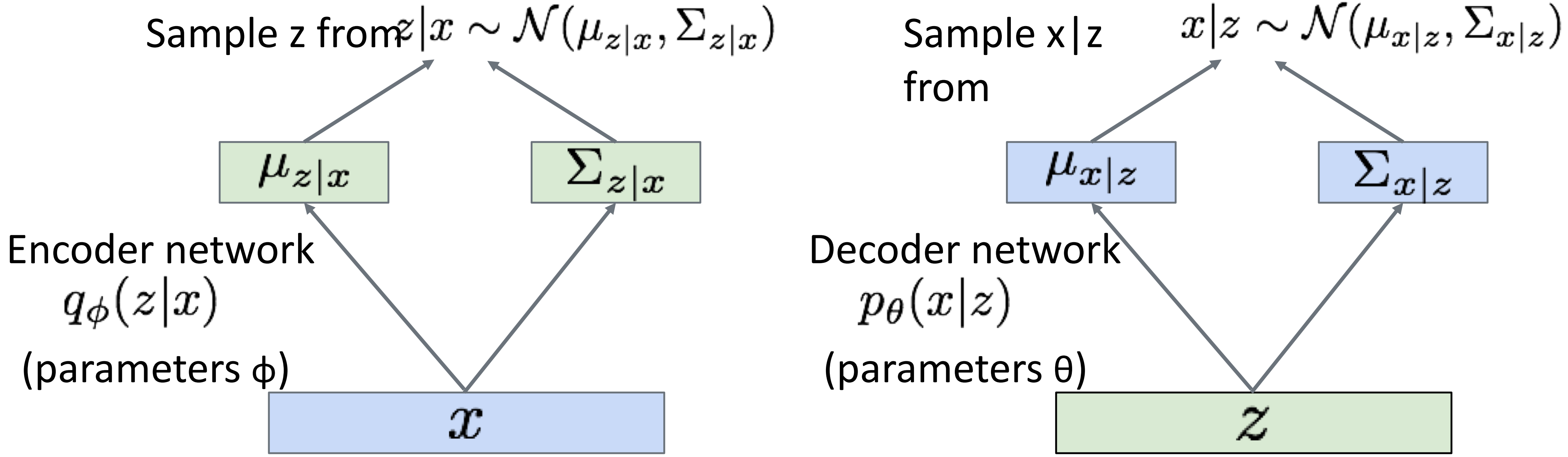

Encoder and decoder networks also called "recognition"/"inference" and "generation" networks

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Slide credit: Fei-Fei Li, Justin Johnson, Serena Yeung

Variational Autoencoders

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

$$\log p_\theta(x^{(i)}) = \mathbf{E}_{z \sim q_\phi(z|x^{(i)})} \left[\log p_\theta(x^{(i)}) \right] \qquad (p_\theta(x^{(i)}) \text{ Does not depend on } z)$$

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Taking expectation wrt. z (using encoder network) will come in handy later

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$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z) p_\theta(z)}{p_\theta(z \mid x^{(i)})}\right] \qquad \text{(Bayes' Rule)}$$

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$$= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z)}\right] + \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z \mid x^{(i)})}\right] \qquad \text{(Logarithms)}$$

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\end{aligned}
$$

The expectation wrt. z
(using encoder network)
let us write nice KL terms

Slide credit: Fei-Fei Li, Justin Johnson, Serena Yeung

Variational Autoencoders

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$$

Decoder network gives $p_\theta(x|z)$, can compute estimate of this term through sampling. (Sampling differentiable through reparam. trick, see paper.)

This KL term (between Gaussians for encoder and z prior) has nice closed-form solution!

$p_\theta(z|x)$ intractable (saw earlier), can't compute this KL term :(But we know KL divergence always >= 0.

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Variational Autoencoders

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We want to maximize the data likelihood

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We want to maximize the data likelihood

Tractable lower bound which we can take gradient of and optimize! ($p_\theta(x|z)$ differentiable, KL term differentiable)

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$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\frac{q_\phi(z \mid x^{(i)})}{q_\phi(z \mid x^{(i)})}\right] \qquad \text{(Multiply by constant)}$$

$$= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z)}\right] + \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z \mid x^{(i)})}\right] \qquad \text{(Logarithms)}$$

$$= \underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)},\theta,\phi)} + \underbrace{D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z \mid x^{(i)}))}_{\geq 0}$$

$$\boxed{\log p_\theta(x^{(i)}) \geq \mathcal{L}(x^{(i)},\theta,\phi)}$$

Variational lower bound ("ELBO")

$$\boxed{\theta^*, \phi^* = \arg\max_{\theta,\phi} \sum_{i=1}^{N} \mathcal{L}(x^{(i)},\theta,\phi)}$$

Training: Maximize lower bound

Variational Autoencoders

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

$$\log p_\theta(x^{(i)}) = \mathbf{E}_{z\sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \qquad (p_\theta(x^{(i)}) \text{ Does not depend on } z)$$

$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\right] \qquad \text{(Bayes' Rule)}$$

$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\frac{q_\phi(z \mid x^{(i)})}{q_\phi(z \mid x^{(i)})}\right] \qquad \text{(Multiply by constant)}$$

$$= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z)}\right] + \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z \mid x^{(i)})}\right] \qquad \text{(Logarithms)}$$

$$= \underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)},\theta,\phi)} + \underbrace{D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z \mid x^{(i)}))}_{\geq 0}$$

Reconstruct the input data

Make approximate posterior distribution close to prior

$$\log p_\theta(x^{(i)}) \geq \mathcal{L}(x^{(i)},\theta,\phi)$$

Variational lower bound ("ELBO")

$$\theta^*, \phi^* = \arg\max_{\theta,\phi} \sum_{i=1}^{N} \mathcal{L}(x^{(i)},\theta,\phi)$$

Training: Maximize lower bound

Slide credit: Fei-Fei Li, Justin Johnson, Serena Yeung

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)},\theta,\phi)}$$

Input Data x

Slide credit: Fei-Fei Li, Justin Johnson, Serena Yeung

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)},\theta,\phi)}$$

Let's look at computing the bound (forward pass) for a given minibatch of input data

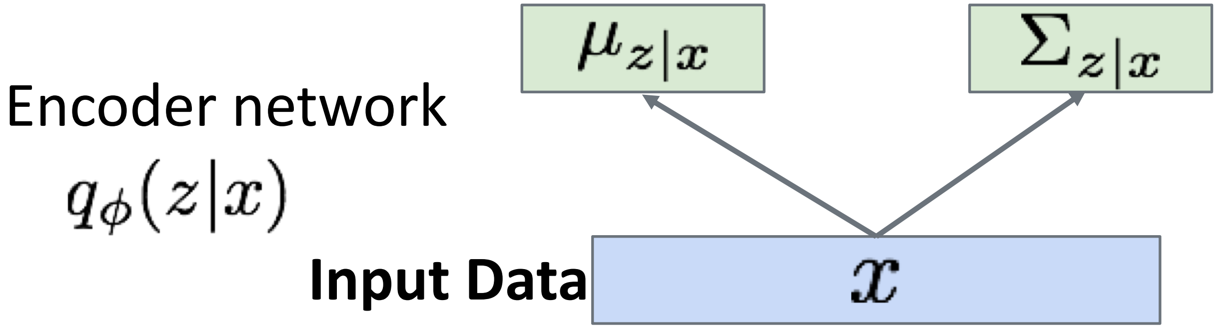
Input Data x

Slide credit: Fei-Fei Li, Justin Johnson, Serena Yeung

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)},\theta,\phi)}$$



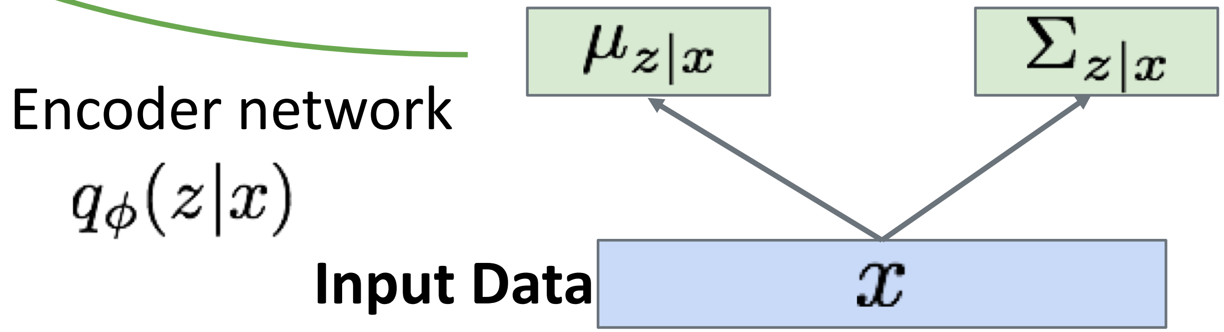
Slide credit: Fei-Fei Li, Justin Johnson, Serena Yeung

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

Make approximate posterior distribution close to prior



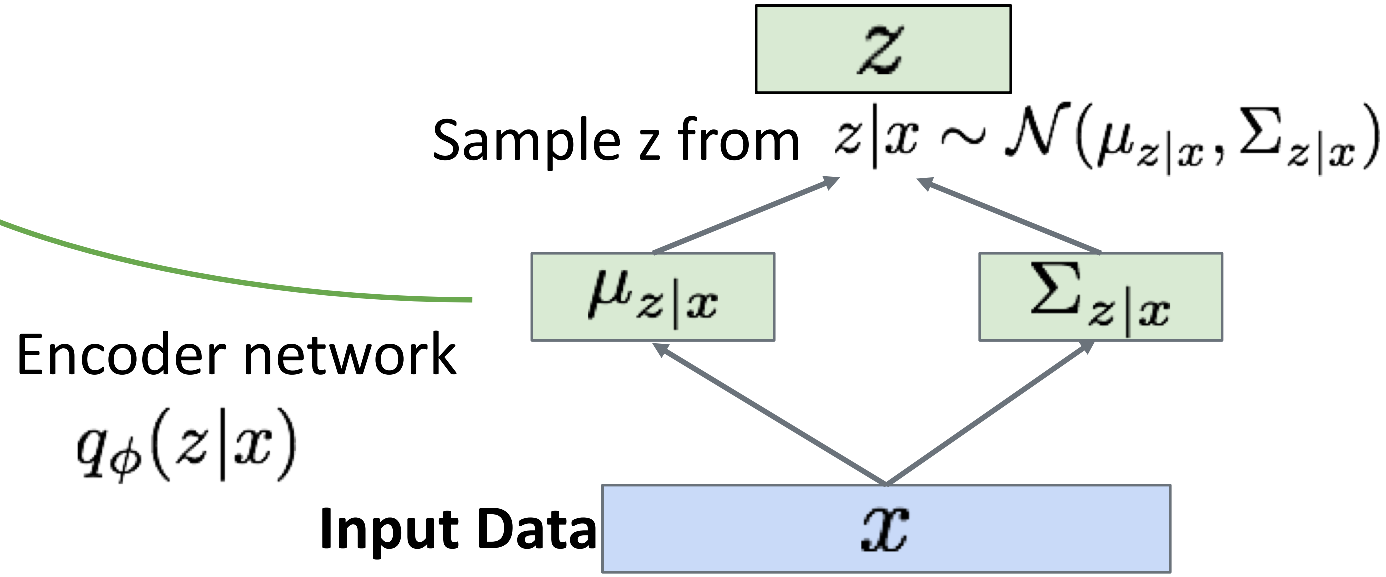
Slide credit: Fei-Fei Li, Justin Johnson, Serena Yeung

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)},\theta,\phi)}$$

Make approximate posterior distribution close to prior



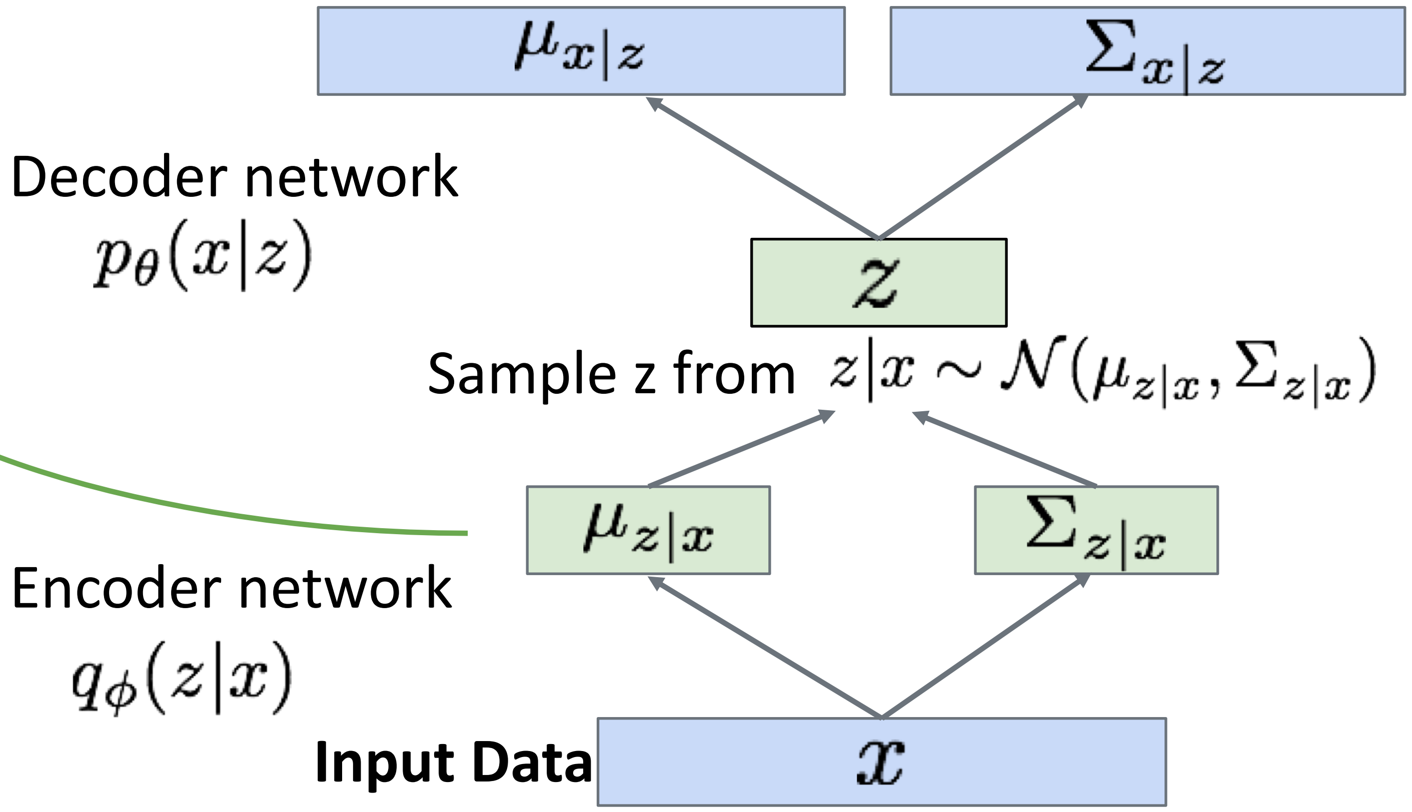
Slide credit: Fei-Fei Li, Justin Johnson, Serena Yeung

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)},\theta,\phi)}$$

Make approximate posterior distribution close to prior



Slide credit: Fei-Fei Li, Justin Johnson, Serena Yeung

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

Maximize likelihood of original input being reconstructed

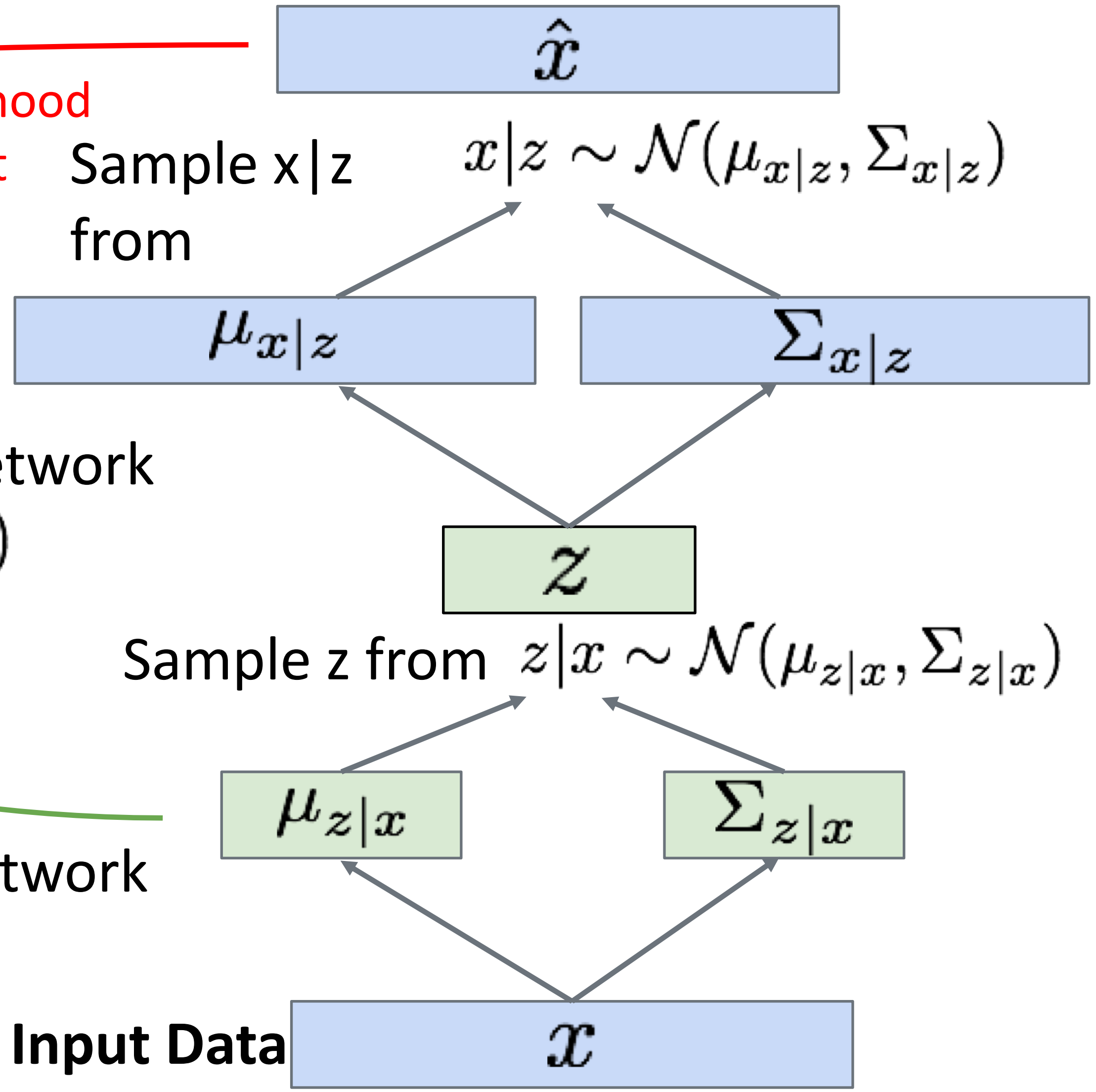
Make approximate posterior distribution close to prior

Decoder network

$p_\theta(x|z)$

Encoder network

$q_\phi(z|x)$



Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

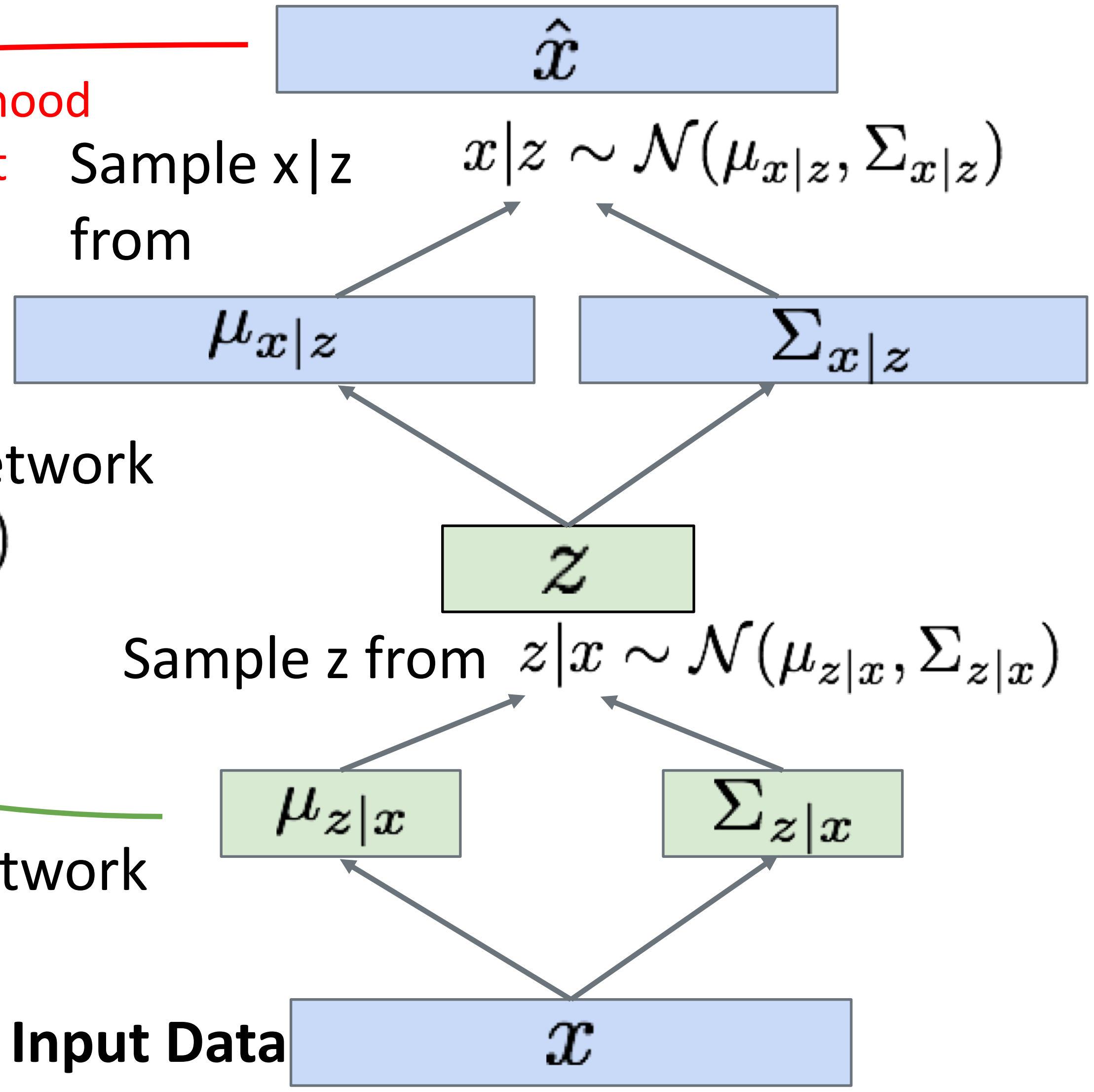
$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)},\theta,\phi)}$$

Maximize likelihood of original input being reconstructed

Make approximate posterior distribution close to prior

Decoder network $p_\theta(x|z)$

Encoder network $q_\phi(z|x)$

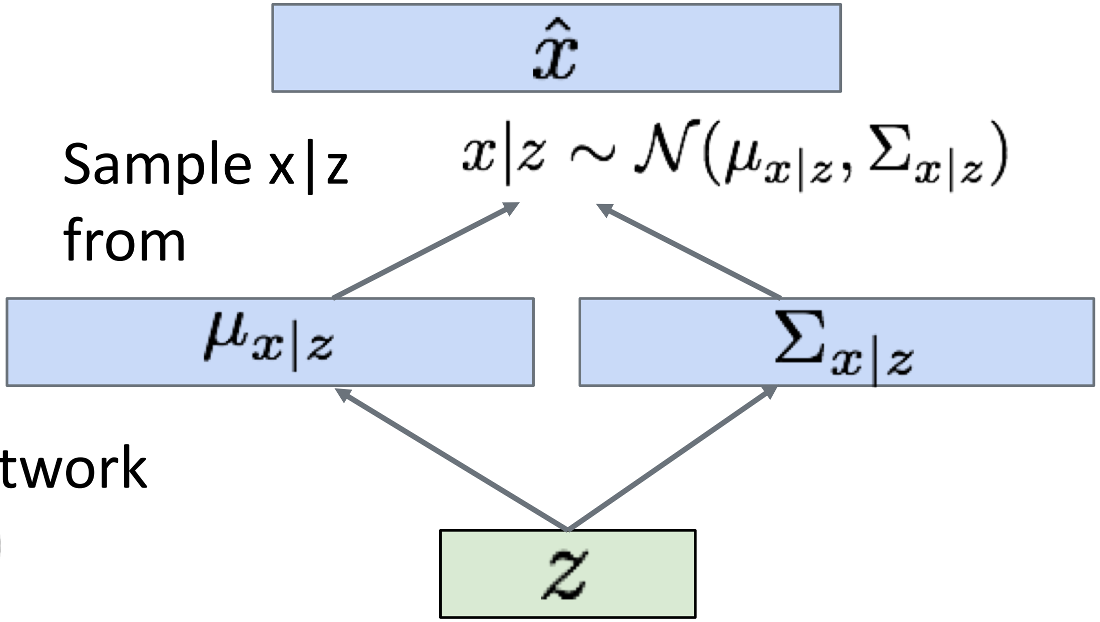


For every minibatch of input data: compute this forward pass, and then backprop!

Slide credit: Fei-Fei Li, Justin Johnson, Serena Yeung

Variational Autoencoders: Generating Data!

Use decoder network. Now sample z from prior!



Decoder network
$p_\theta(x|z)$

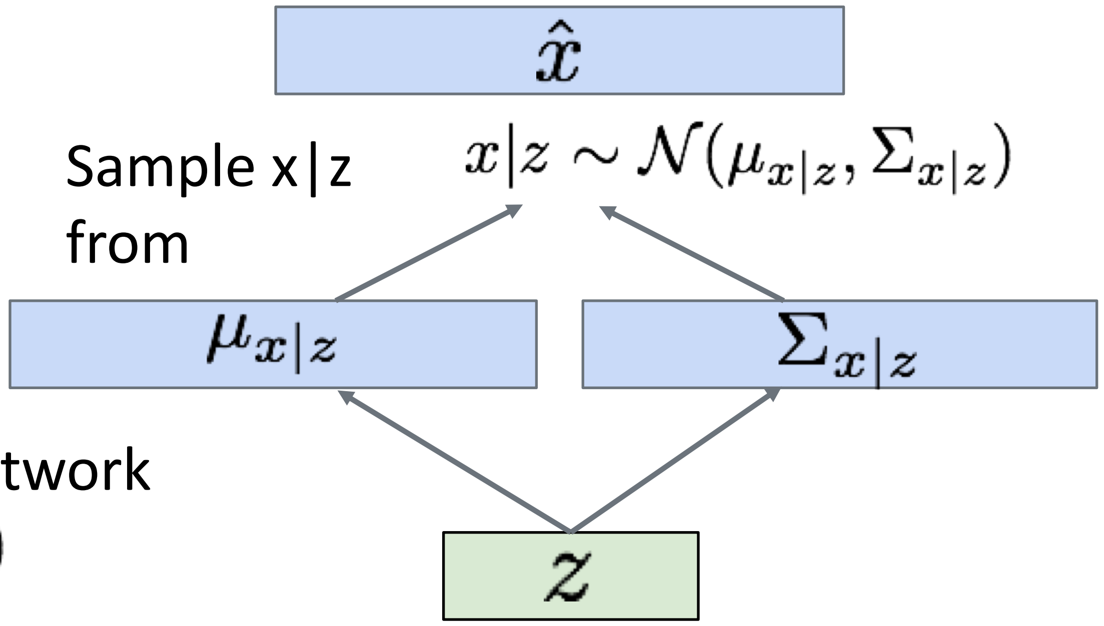
Sample z from $z \sim \mathcal{N}(0, I)$

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders: Generating Data!

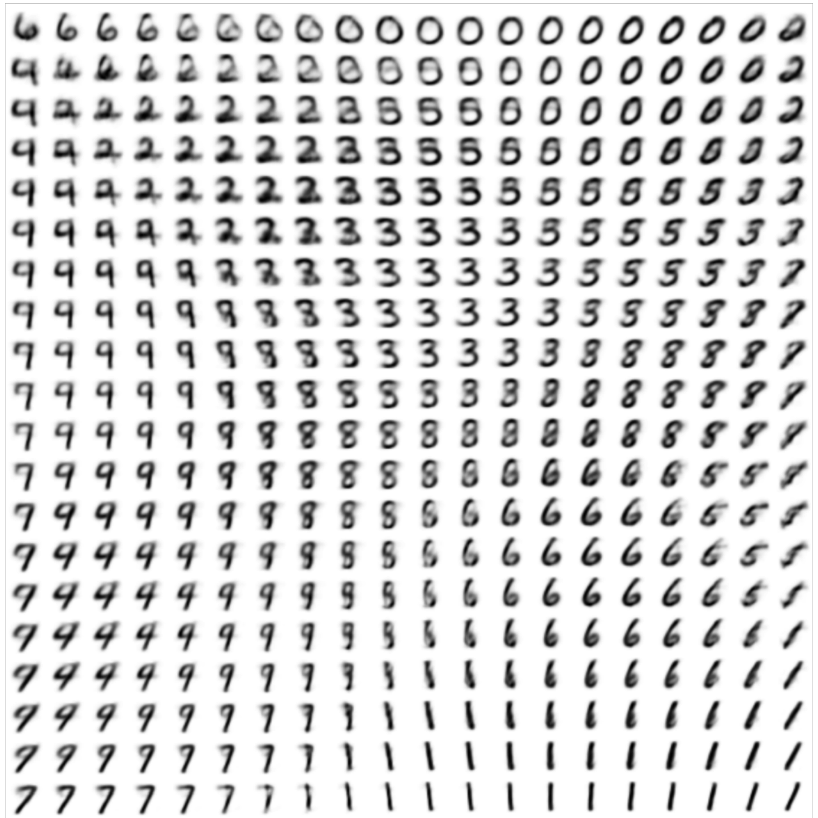
Use decoder network. Now sample z from prior!

Sample x|z from $x|z \sim \mathcal{N}(\mu_{x|z}, \Sigma_{x|z})$



Decoder network $p_\theta(x|z)$

Sample z from $z \sim \mathcal{N}(0, I)$



Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Slide credit: Fei-Fei Li, Justin Johnson, Serena Yeung

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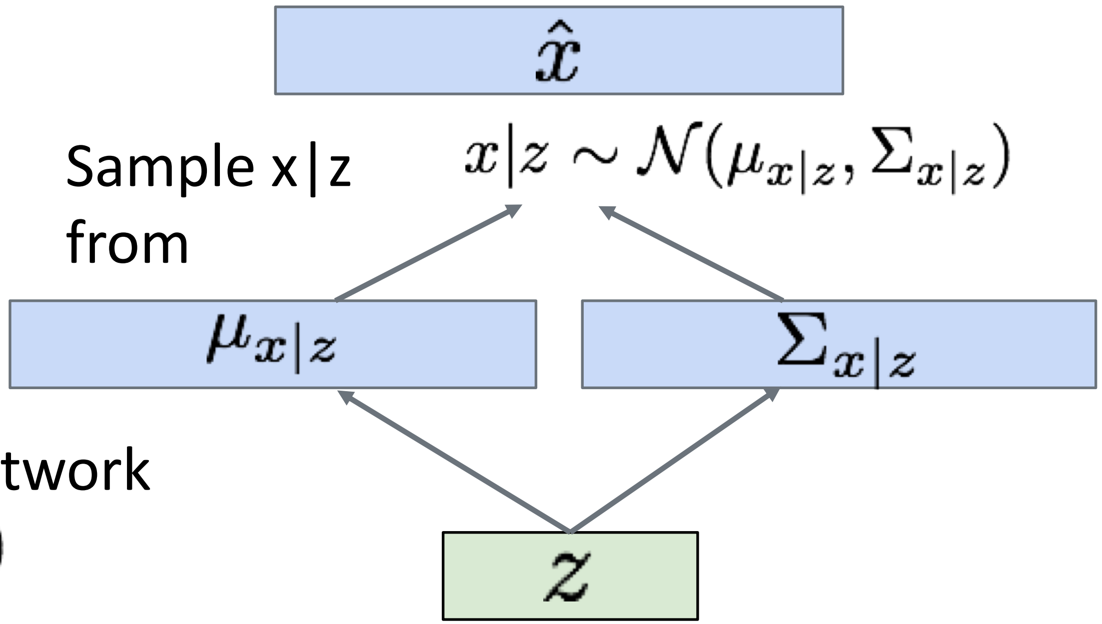
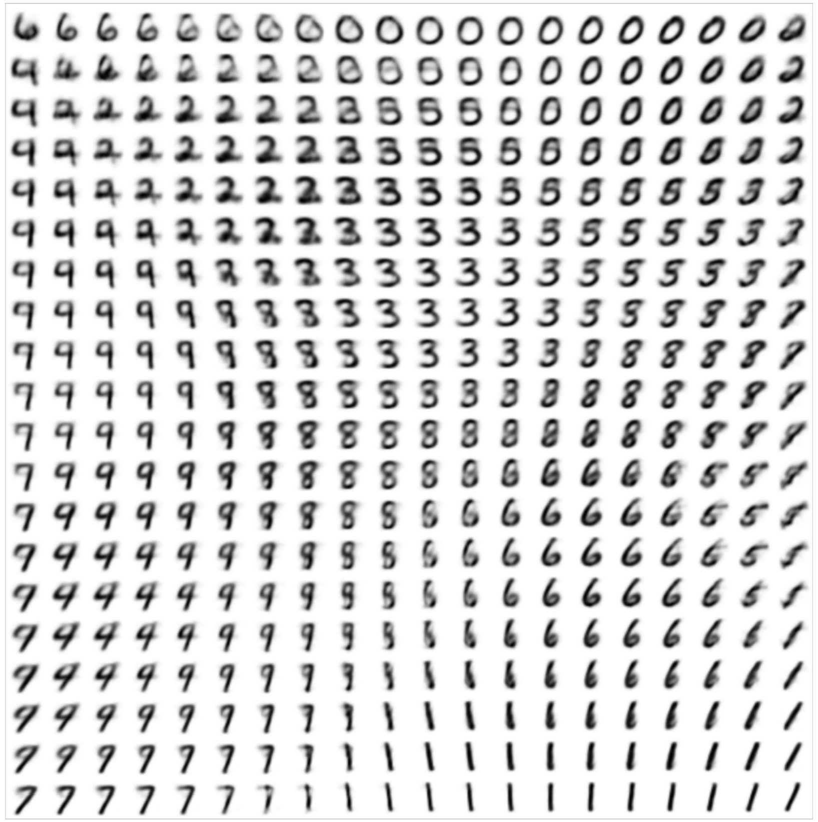


Decoder network
$p_\theta(x|z)$

Sample z from $z \sim \mathcal{N}(0, I)$

Data manifold for 2-d **z**

Vary $\mathbf{z_1}$



Vary $\mathbf{z_2}$

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Slide credit: Fei-Fei Li, Justin Johnson, Serena Yeung

Variational Autoencoders: Generating Data!

Diagonal prior on **z** => independent latent variables

Different dimensions of **z** encode interpretable factors of variation

Degree of smile

Vary $\mathbf{z_1}$

Vary $\mathbf{z_2}$

Head pose

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders: Generating Data!

Diagonal prior on **z** => independent latent variables

Different dimensions of **z** encode interpretable factors of variation

Degree of smile

Vary $\mathbf{z_1}$

Vary $\mathbf{z_2}$

Head pose

Also good feature representation that can be computed using $q_\phi(z|x)$!

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Slide credit: Fei-Fei Li, Justin Johnson, Serena Yeung

Variational Autoencoders: Generating Data!

32x32 CIFAR-10

Labeled Faces in the Wild

Slide credit: Fei-Fei Li, Justin Johnson, Serena Yeung