

# UC Berkeley · CSW182 | [Deep Learning]

## Designing, Visualizing and Understanding Deep Neural Networks (2021)

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# Latent Variable Models

Designing, Visualizing and Understanding Deep Neural Networks

CS W182/282A

Instructor: Sergey Levine  
UC Berkeley

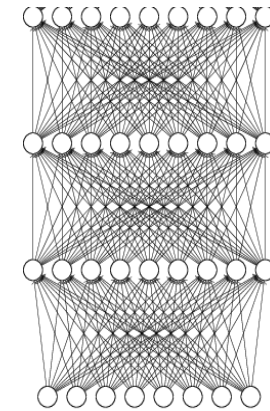
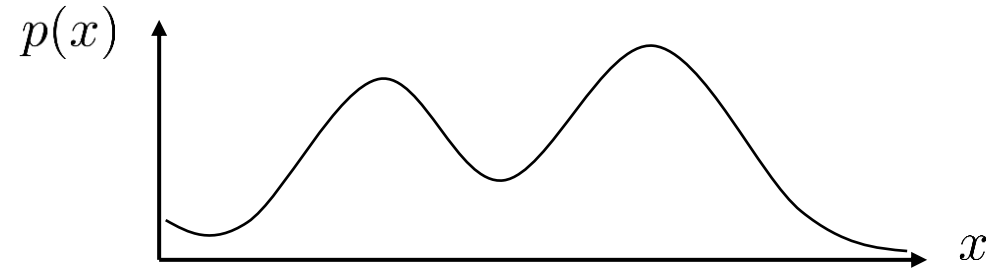


# Latent variable models in general

$$p(x) = \int p(x|z)p(z)dz$$

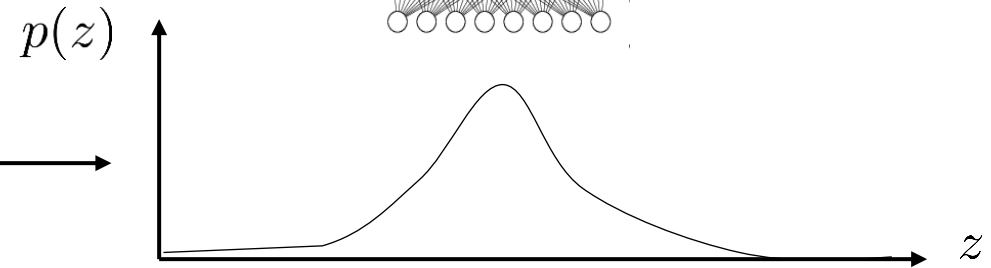
“easy” distribution  
(e.g., conditional Gaussian)

“easy” distribution  
(e.g., Gaussian)



$$p(x|z) = \mathcal{N}(\mu_{\text{nn}}(z), \sigma_{\text{nn}}(z))$$

“easy” distribution  
(e.g., Gaussian)



# Estimating the log-likelihood

*expected* log-likelihood:

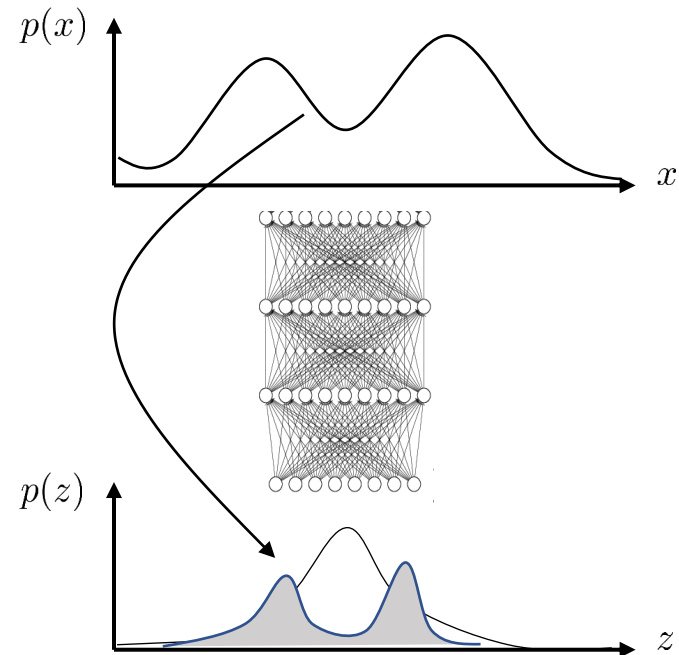
$$\theta \leftarrow \arg \max_{\theta} \frac{1}{N} \sum_i E_{z \sim p(z|x_i)} [\log p_{\theta}(x_i, z)]$$

but... how do we calculate  $p(z|x_i)$ ?

this is called **probabilistic inference**

intuition: “guess” most likely  $z$  given  $x_i$ ,  
and pretend it’s the right one

...but there are many possible values of  $z$   
so use the distribution  $p(z|x_i)$



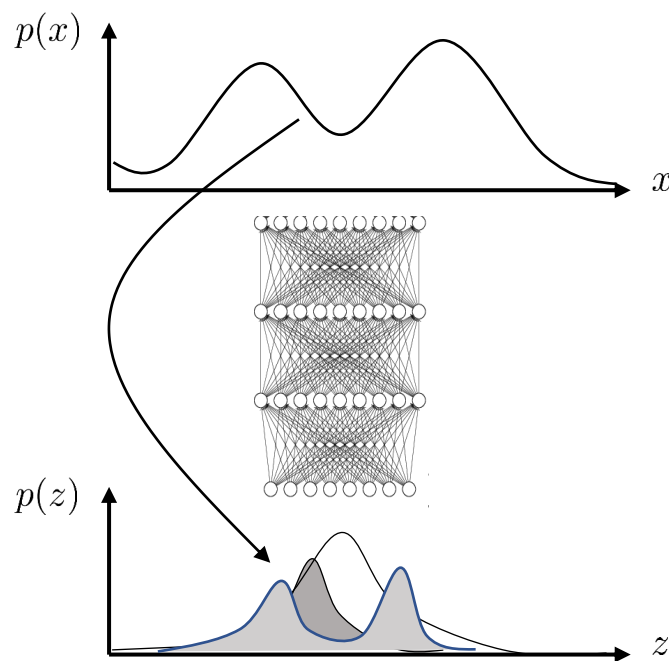
# The variational approximation

but... how do we calculate  $p(z|x_i)$ ?

what if we approximate with  $q_i(z) = \mathcal{N}(\mu_i, \sigma_i)$

can bound  $\log p(x_i)$ !

$$\begin{aligned}\log p(x_i) &= \log \int_z p(x_i|z)p(z) \\ &= \log \int_z p(x_i|z)p(z) \frac{q_i(z)}{q_i(z)} \\ &= \log E_{z \sim q_i(z)} \left[ \frac{p(x_i|z)p(z)}{q_i(z)} \right]\end{aligned}$$



# The variational approximation

but... how do we calculate  $p(z|x_i)$ ?

can bound  $\log p(x_i)$ !

$$\log p(x_i) = \log \int_z p(x_i|z)p(z)$$

$$= \log \int_z p(x_i|z)p(z) \frac{q_i(z)}{q_i(z)}$$

$$= \log E_{z \sim q_i(z)} \left[ \frac{p(x_i|z)p(z)}{q_i(z)} \right]$$

$$\geq E_{z \sim q_i(z)} \left[ \log \frac{p(x_i|z)p(z)}{q_i(z)} \right] = E_{z \sim q_i(z)} [\log p(x_i|z) + \log p(z)] + E_{z \sim q_i(z)} [\log q_i(z)]$$

Jensen's inequality

$$\log E[y] \geq E[\log y]$$

maximizing this maximizes  $\log p(x_i)$



# A brief aside...

## Entropy:

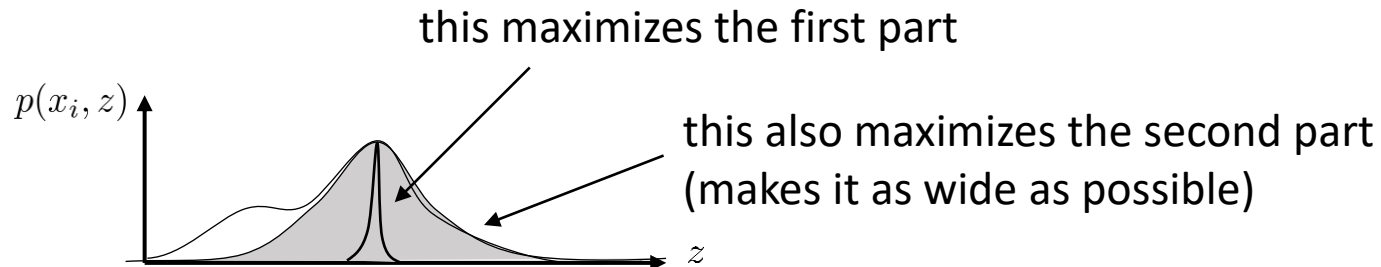
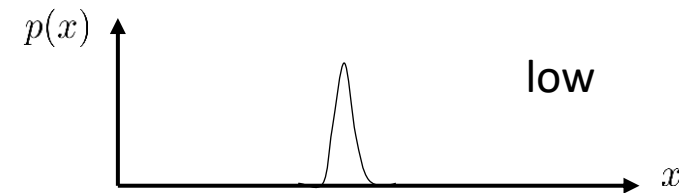
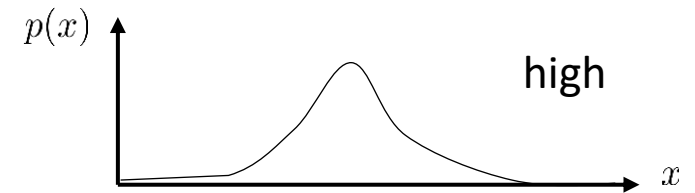
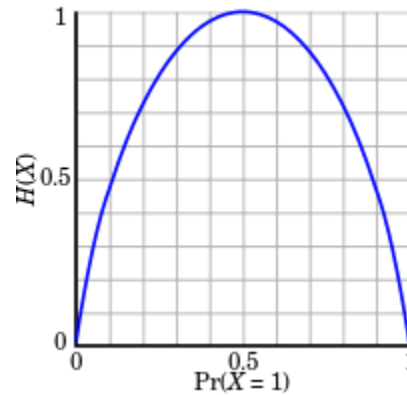
$$\mathcal{H}(p) = -E_{x \sim p(x)}[\log p(x)] = - \int_x p(x) \log p(x) dx$$

Intuition 1: how *random* is the random variable?

Intuition 2: how large is the log probability in expectation *under itself*

what do we expect this to do?

$$E_{z \sim q_i(z)}[\log p(x_i|z) + \log p(z)] + \mathcal{H}(q_i)$$



# A brief aside...

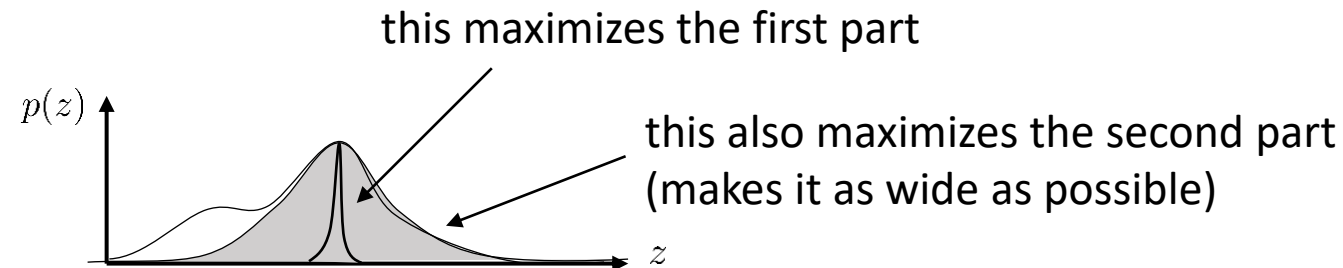
## KL-Divergence:

$$D_{\text{KL}}(q||p) = E_{x \sim q(x)} \left[ \log \frac{q(x)}{p(x)} \right] = E_{x \sim q(x)} [\log q(x)] - E_{x \sim q(x)} [\log p(x)] = -E_{x \sim q(x)} [\log p(x)] - \mathcal{H}(q)$$

Intuition 1: how *different* are two distributions?

Intuition 2: how small is the expected log probability of one distribution under another, minus entropy?

why entropy?





# The variational approximation

$$\log p(x_i) \geq \overbrace{E_{z \sim q_i(z)} [\log p(x_i|z) + \log p(z)]}^{\mathcal{L}_i(p, q_i)} + \mathcal{H}(q_i)$$

what makes a good  $q_i(z)$ ?

intuition:  $q_i(z)$  should approximate  $p(z|x_i)$

approximate in what sense?

compare in terms of KL-divergence:  $D_{\text{KL}}(q_i(z) \| p(z|x))$

why?

$$\begin{aligned} D_{\text{KL}}(q_i(z) \| p(z|x_i)) &= E_{z \sim q_i(z)} \left[ \log \frac{q_i(z)}{p(z|x_i)} \right] = E_{z \sim q_i(z)} \left[ \log \frac{q_i(z)p(x_i)}{p(x_i, z)} \right] \\ &= -E_{z \sim q_i(z)} [\log p(x_i|z) + \log p(z)] + E_{z \sim q_i(z)} [\log q_i(z)] + E_{z \sim q_i(z)} [\log p(x_i)] \\ &= -E_{z \sim q_i(z)} [\log p(x_i|z) + \log p(z)] - \mathcal{H}(q_i) + \log p(x_i) \\ &= -\mathcal{L}_i(p, q_i) + \log p(x_i) \end{aligned}$$

$$\log p(x_i) = D_{\text{KL}}(q_i(z) \| p(z|x_i)) + \mathcal{L}_i(p, q_i)$$

$$\log p(x_i) \geq \mathcal{L}_i(p, q_i)$$

# The variational approximation

$$\log p(x_i) \geq \overbrace{E_{z \sim q_i(z)} [\log p(x_i|z) + \log p(z)]}^{\mathcal{L}_i(p, q_i)} + \mathcal{H}(q_i)$$

$$\log p(x_i) = D_{\text{KL}}(q_i(z) \| p(z|x_i)) + \mathcal{L}_i(p, q_i)$$

$$\log p(x_i) \geq \mathcal{L}_i(p, q_i)$$

$$\begin{aligned} D_{\text{KL}}(q_i(z) \| p(z|x_i)) &= E_{z \sim q_i(z)} \left[ \log \frac{q_i(z)}{p(z|x_i)} \right] = E_{z \sim q_i(z)} \left[ \log \frac{q_i(z)p(x_i)}{p(x_i, z)} \right] \\ &= \underbrace{-E_{z \sim q_i(z)} [\log p(x_i|z) + \log p(z)]}_{-\mathcal{L}_i(p, q_i)} + \log p(x_i) \end{aligned}$$

independent of  $q_i$ !

$\Rightarrow$  maximizing  $\mathcal{L}_i(p, q_i)$  w.r.t.  $q_i$  minimizes KL-divergence!

# How do we use this?

$$\log p(x_i) \geq \overbrace{E_{z \sim q_i(z)} [\log p_\theta(x_i|z) + \log p(z)]}^{\mathcal{L}_i(p, q_i)} + \mathcal{H}(q_i)$$

~~$$\theta \leftarrow \arg \max_{\theta} \frac{1}{N} \sum_i \log p_\theta(x_i)$$~~

$$\theta \leftarrow \arg \max_{\theta} \frac{1}{N} \sum_i \mathcal{L}_i(p, q_i)$$

for each  $x_i$  (or mini-batch):

calculate  $\nabla_{\theta} \mathcal{L}_i(p, q_i)$ :

sample  $z \sim q_i(z)$

$$\nabla_{\theta} \mathcal{L}_i(p, q_i) \approx \nabla_{\theta} \log p_{\theta}(x_i|z)$$

$$\theta \leftarrow \theta + \alpha \nabla_{\theta} \mathcal{L}_i(p, q_i)$$

update  $q_i$  to maximize  $\mathcal{L}_i(p, q_i)$

let's say  $q_i(z) = \mathcal{N}(\mu_i, \sigma_i)$

use gradient  $\nabla_{\mu_i} \mathcal{L}_i(p, q_i)$  and  $\nabla_{\sigma_i} \mathcal{L}_i(p, q_i)$

gradient ascent on  $\mu_i, \sigma_i$

how?

# What's the problem?

for each  $x_i$  (or mini-batch):

calculate  $\nabla_{\theta} \mathcal{L}_i(p, q_i)$ :

sample  $z \sim q_i(z)$

$$\nabla_{\theta} \mathcal{L}_i(p, q_i) \approx \nabla_{\theta} \log p_{\theta}(x_i|z)$$

$$\theta \leftarrow \theta + \alpha \nabla_{\theta} \mathcal{L}_i(p, q_i)$$

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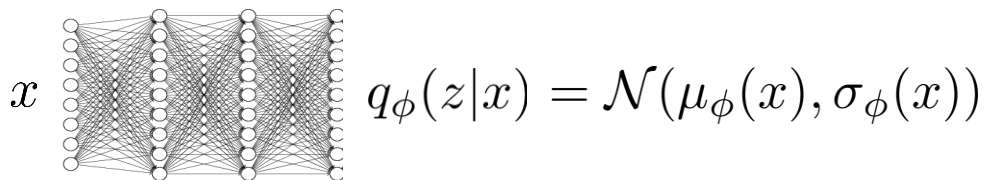
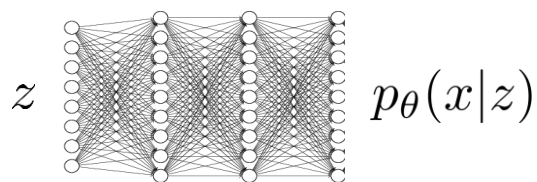
gradient ascent on  $\mu_i, \sigma_i$

How many parameters are there?

$$|\theta| + (|\mu_i| + |\sigma_i|) \times N$$

intuition:  $q_i(z)$  should approximate  $p(z|x_i)$

what if we learn a *network*  $q_i(z) = q(z|x_i) \approx p(z|x_i)$ ?



# Amortized Variational Inference

# What's the problem?

for each  $x_i$  (or mini-batch):

calculate  $\nabla_{\theta} \mathcal{L}_i(p, q_i)$ :

sample  $z \sim q_i(z)$

$$\nabla_{\theta} \mathcal{L}_i(p, q_i) \approx \nabla_{\theta} \log p_{\theta}(x_i|z)$$

$$\theta \leftarrow \theta + \alpha \nabla_{\theta} \mathcal{L}_i(p, q_i)$$

update  $q_i$  to maximize  $\mathcal{L}_i(p, q_i)$

let's say  $q_i(z) = \mathcal{N}(\mu_i, \sigma_i)$

use gradient  $\nabla_{\mu_i} \mathcal{L}_i(p, q_i)$  and  $\nabla_{\sigma_i} \mathcal{L}_i(p, q_i)$

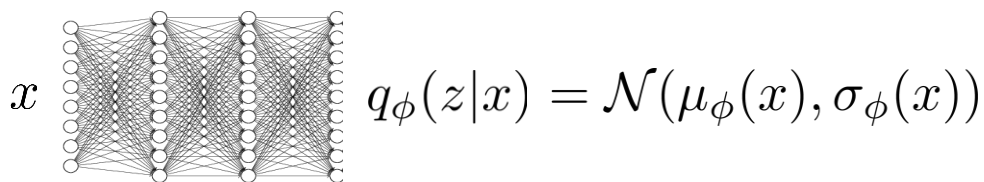
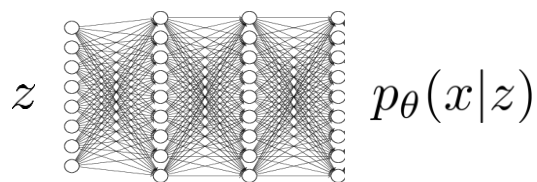
gradient ascent on  $\mu_i, \sigma_i$

How many parameters are there?

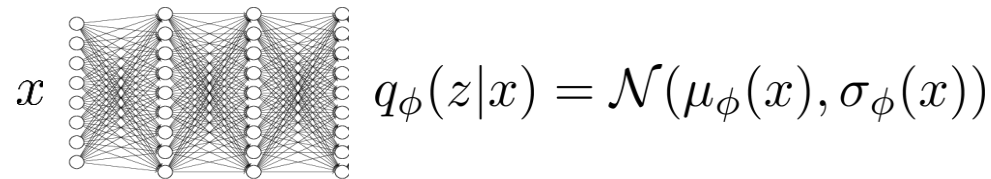
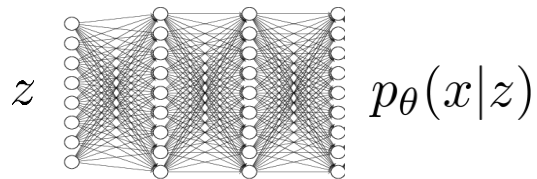
$$|\theta| + (|\mu_i| + |\sigma_i|) \times N$$

intuition:  $q_i(z)$  should approximate  $p(z|x_i)$

what if we learn a *network*  $q_i(z) = q(z|x_i) \approx p(z|x_i)$ ?



# Amortized variational inference



for each  $x_i$  (or mini-batch):

calculate  $\nabla_\theta \mathcal{L}(p_\theta(x_i|z), q_\phi(z|x_i))$ :

sample  $z \sim q_\phi(z|x_i)$

$\nabla_\theta \mathcal{L} \approx \nabla_\theta \log p_\theta(x_i|z)$

$\theta \leftarrow \theta + \alpha \nabla_\theta \mathcal{L}$

$\phi \leftarrow \phi + \alpha \nabla_\phi \mathcal{L}$

how do we calculate this?

$$\log p(x_i) \geq \overbrace{E_{z \sim q_\phi(z|x_i)} [\log p_\theta(x_i|z) + \log p(z)]}^{\mathcal{L}(p_\theta(x_i|z), q_\phi(z|x_i))} + \mathcal{H}(q_\phi(z|x_i))$$

# Amortized variational inference

for each  $x_i$  (or mini-batch):

calculate  $\nabla_{\theta} \mathcal{L}(p_{\theta}(x_i|z), q_{\phi}(z|x_i))$ :

sample  $z \sim q_{\phi}(z|x_i)$

$\nabla_{\theta} \mathcal{L} \approx \nabla_{\theta} \log p_{\theta}(x_i|z)$

$\theta \leftarrow \theta + \alpha \nabla_{\theta} \mathcal{L}$

$\phi \leftarrow \phi + \alpha \nabla_{\phi} \mathcal{L}$

$$q_{\phi}(z|x) = \mathcal{N}(\mu_{\phi}(x), \sigma_{\phi}(x))$$

look up formula for  
entropy of a Gaussian



$$\mathcal{L}_i = \underbrace{E_{z \sim q_{\phi}(z|x_i)} [\log p_{\theta}(x_i|z) + \log p(z)]}_{J(\phi)} + \mathcal{H}(q_{\phi}(z|x_i))$$

$$J(\phi) = E_{z \sim q_{\phi}(z|x_i)} [r(x_i, z)]$$

can just use policy gradient!

What's wrong with this gradient?

$$\nabla J(\phi) \approx \frac{1}{M} \sum_j \nabla_{\phi} \log q_{\phi}(z_j|x_i) r(x_i, z_j)$$



# The reparameterization trick

Is there a better way?

$$\begin{aligned} J(\phi) &= E_{z \sim q_\phi(z|x_i)}[r(x_i, z)] \\ &= E_{\epsilon \sim \mathcal{N}(0,1)}[r(x_i, \mu_\phi(x_i) + \epsilon \sigma_\phi(x_i))] \end{aligned}$$

estimating  $\nabla_\phi J(\phi)$ :

sample  $\epsilon_1, \dots, \epsilon_M$  from  $\mathcal{N}(0, 1)$  (a single sample works well!)

$$\nabla_\phi J(\phi) \approx \frac{1}{M} \sum_j \nabla_\phi r(x_i, \mu_\phi(x_i) + \epsilon_j \sigma_\phi(x_i))$$

most autodiff software (e.g., TensorFlow)  
will compute this for you!

$$q_\phi(z|x) = \mathcal{N}(\mu_\phi(x), \sigma_\phi(x))$$

$$z = \mu_\phi(x) + \epsilon \sigma_\phi(x)$$

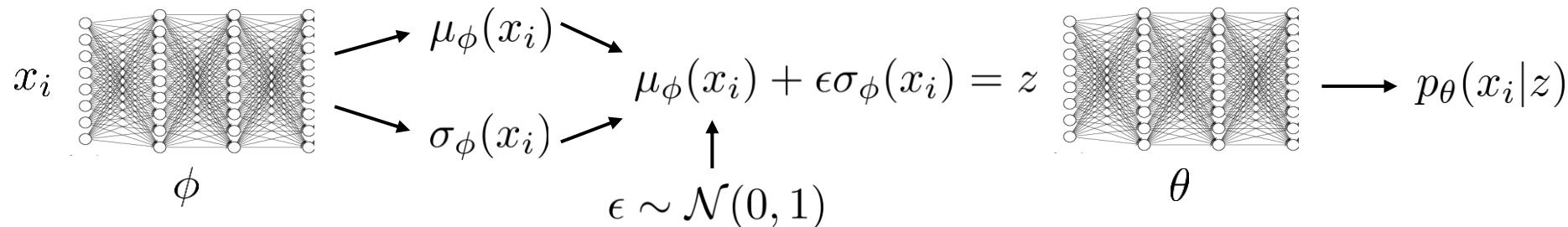


$$\epsilon \sim \mathcal{N}(0, 1)$$

independent of  $\phi$ !

# Another way to look at it...

$$\begin{aligned}\mathcal{L}_i &= E_{z \sim q_\phi(z|x_i)} [\log p_\theta(x_i|z) + \log p(z)] + \mathcal{H}(q_\phi(z|x_i)) \\ &= E_{z \sim q_\phi(z|x_i)} [\log p_\theta(x_i|z)] + \underbrace{E_{z \sim q_\phi(z|x_i)} [\log p(z)] + \mathcal{H}(q_\phi(z|x_i))}_{-D_{\text{KL}}(q_\phi(z|x_i) \| p(z))} \leftarrow \text{this often has a convenient analytical form (e.g., KL-divergence for Gaussians)} \\ &= E_{z \sim q_\phi(z|x_i)} [\log p_\theta(x_i|z)] - D_{\text{KL}}(q_\phi(z|x_i) \| p(z)) \\ &= E_{\epsilon \sim \mathcal{N}(0,1)} [\log p_\theta(x_i | \mu_\phi(x_i) + \epsilon \sigma_\phi(x_i))] - D_{\text{KL}}(q_\phi(z|x_i) \| p(z)) \\ &\approx \log p_\theta(x_i | \mu_\phi(x_i) + \epsilon \sigma_\phi(x_i)) - D_{\text{KL}}(q_\phi(z|x_i) \| p(z))\end{aligned}$$



# Reparameterization trick vs. policy gradient

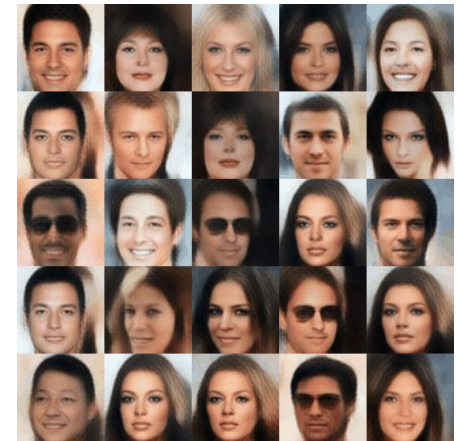
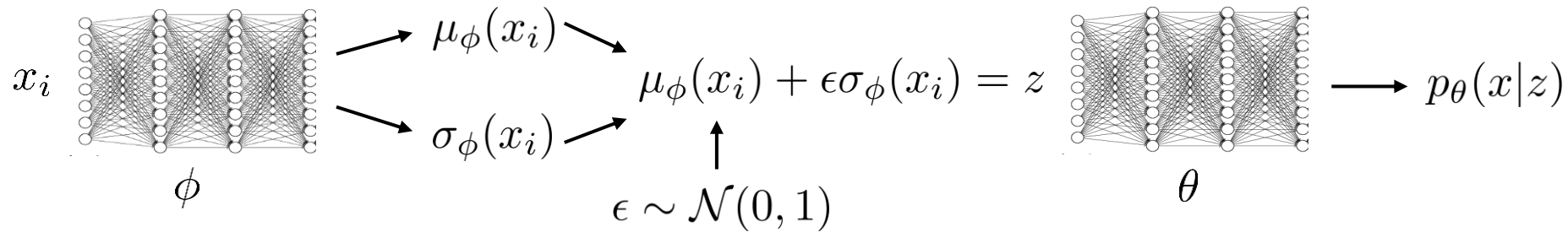
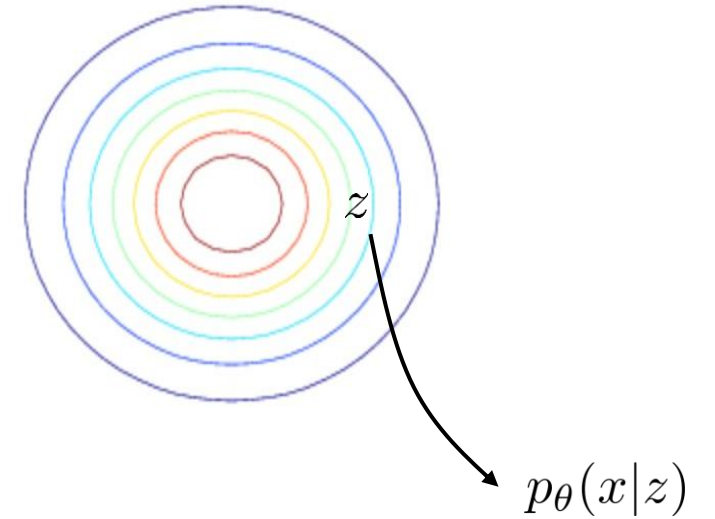
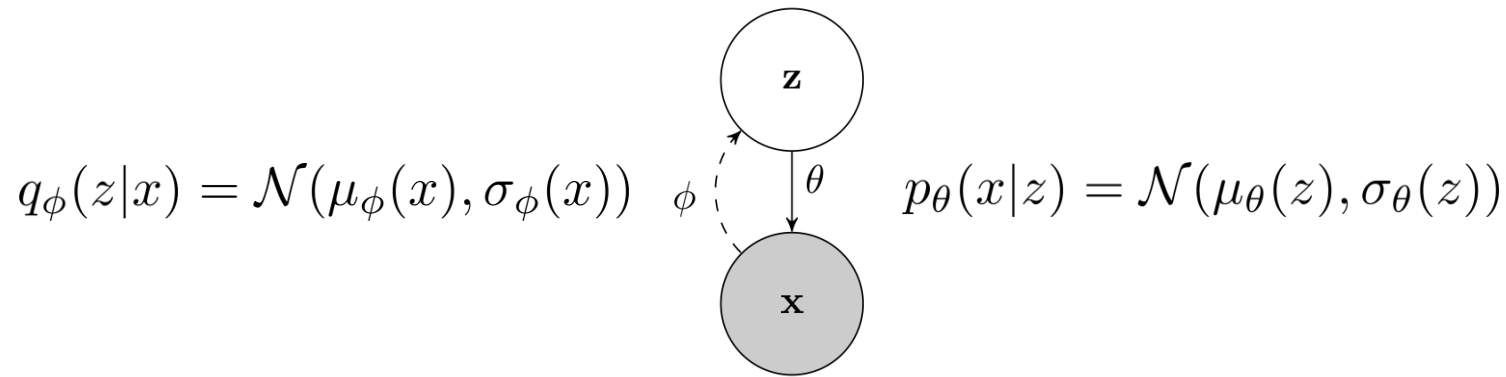
- Policy gradient
  - Can handle both discrete and continuous latent variables
  - High variance, requires multiple samples & small learning rates
- Reparameterization trick
  - Only continuous latent variables
  - Very simple to implement
  - Low variance

$$J(\phi) \approx \frac{1}{M} \sum_j \nabla_{\phi} \log q_{\phi}(z_j|x_i) r(x_i, z_j)$$

$$\nabla_{\phi} J(\phi) \approx \frac{1}{M} \sum_j \nabla_{\phi} r(x_i, \mu_{\phi}(x_i) + \epsilon_j \sigma_{\phi}(x_i))$$

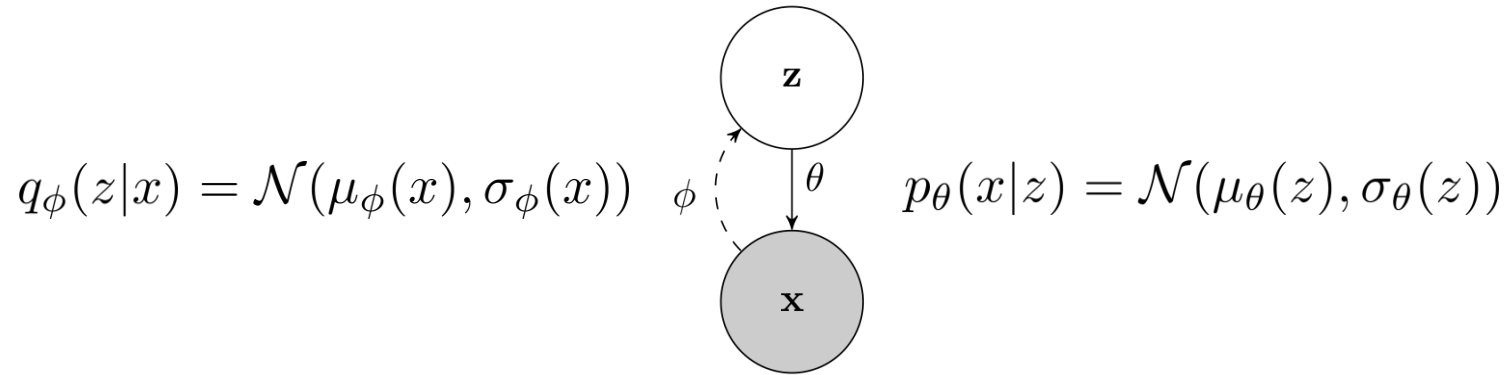
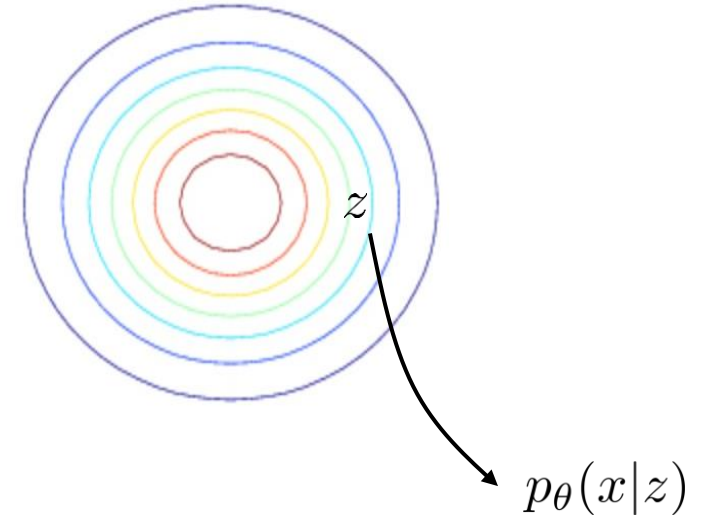
# Variational Autoencoders

# The *variational* autoencoder



$$\max_{\theta, \phi} \frac{1}{N} \sum_i \log p_{\theta}(x_i | \mu_{\phi}(x_i) + \epsilon \sigma_{\phi}(x_i)) - D_{\text{KL}}(q_{\phi}(z|x_i) \| p(z))$$

# Using the variational autoencoder



$$p(x) = \int p(x|z)p(z)dz$$

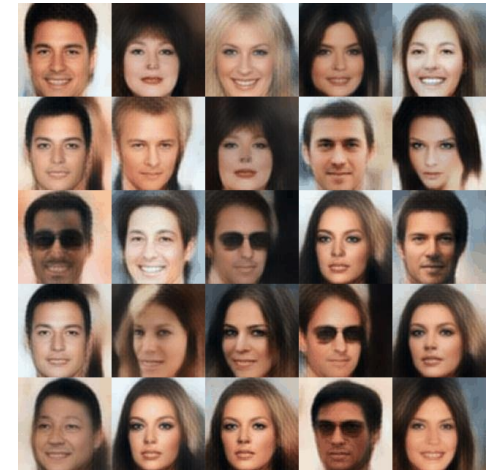
why does this work?

sampling:

$$z \sim p(z)$$

$$x \sim p(x|z)$$

$$\mathcal{L}_i = E_{z \sim q_\phi(z|x_i)}[\log p_\theta(x_i|z)] - D_{\text{KL}}(q_\phi(z|x_i) || p(z))$$



# Conditional models

$$\mathcal{L}_i = E_{z \sim q_\phi(z|x_i, y_i)} [\log p_\theta(y_i|x_i, z) + \log p(z|x_i)] + \mathcal{H}(q_\phi(z|x_i, y_i))$$

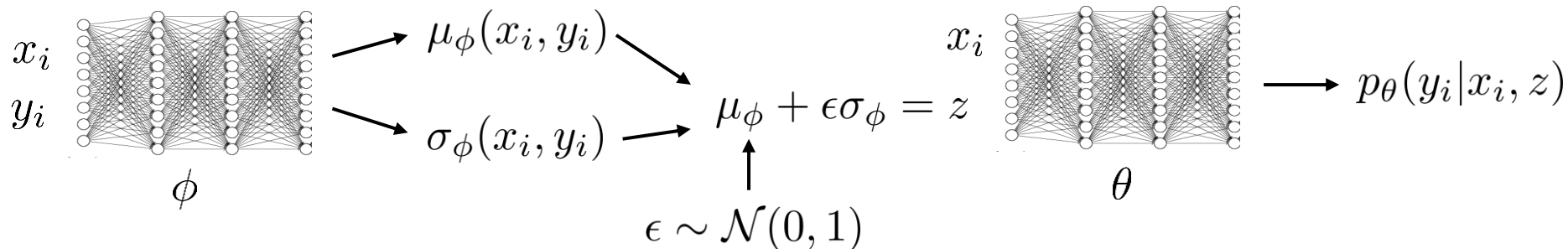
just like before, only now generating  $y_i$   
and *everything* is conditioned on  $x_i$

at test time:

$$z \sim p(z|x_i)$$

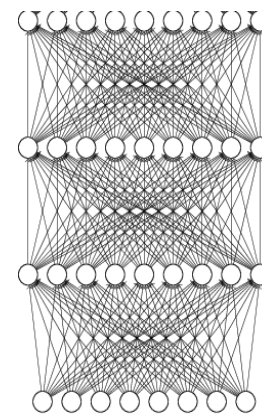
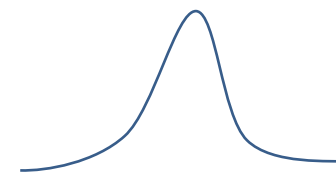
$$y \sim p(y|x_i, z)$$

can *optionally* depend on  $x$



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

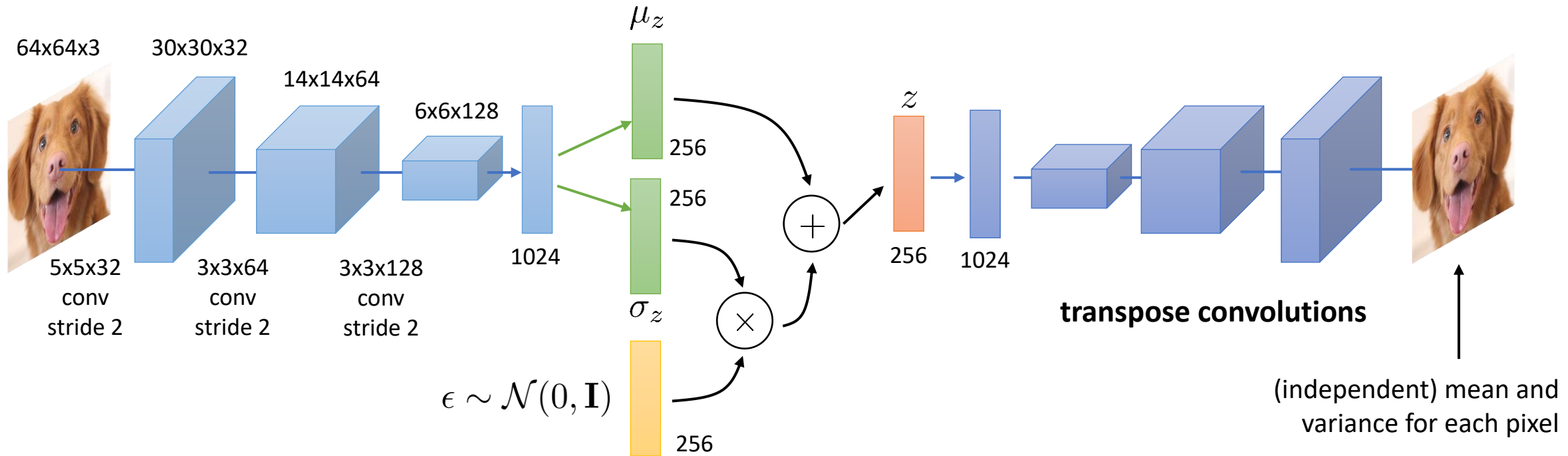
$$p(z)$$



$$p(y|x, z)$$



# VAEs with convolutions



**Question:** can we design a **fully convolutional** VAE?

**Yes,** but be careful with the latent codes!

$p(z) = \mathcal{N}(0, \mathbf{I})$   $\longleftarrow$  implies all  $z$  dimensions are independent



# VAEs in practice

**Common issue:** very tempting for VAEs (especially **conditional** VAEs) to ignore the latent codes, or generate poor samples

↑  
why?

**Problem 1:** latent code is ignored

$$p_{\theta}(x|z) \rightarrow p(x)$$

**what does this look like?**      blurry “average” image  
when *reconstructing*

$$z \sim q_{\phi}(z|x) \quad x \sim p_{\theta}(x|z)$$

**too low**    no info in  $z$

$$D_{\text{KL}}(q_{\phi}(z|x) || p(z))$$

**too high**

too much info in  $z$

↑  
need to control this quantity  
carefully to get good results!

**Problem 2:** latent code is not *compressed*

$$q_{\phi}(z|x) \text{ very far from } p(z)$$

**what does this look like?**      garbage images  
when *sampling*

$$z \sim p(z) \quad x \sim p_{\theta}(x|z)$$

# VAEs in practice

**Problem 1:** latent code is ignored

**too low** no info in  $z$

$$D_{\text{KL}}(q_{\phi}(z|x)||p(z))$$

**Problem 2:** latent code is not *compressed*

**too high** too much info in  $z$



need to control this quantity  
carefully to get good results!

$$\max_{\theta, \phi} \frac{1}{N} \sum_i \log p_{\theta}(x_i | \mu_{\phi}(x_i) + \epsilon \sigma_{\phi}(x_i)) - \beta D_{\text{KL}}(q_{\phi}(z|x_i)||p(z))$$



multiplier to adjust regularizer strength

adjust  $\beta$  manually to get good reconstructions **and** good samples

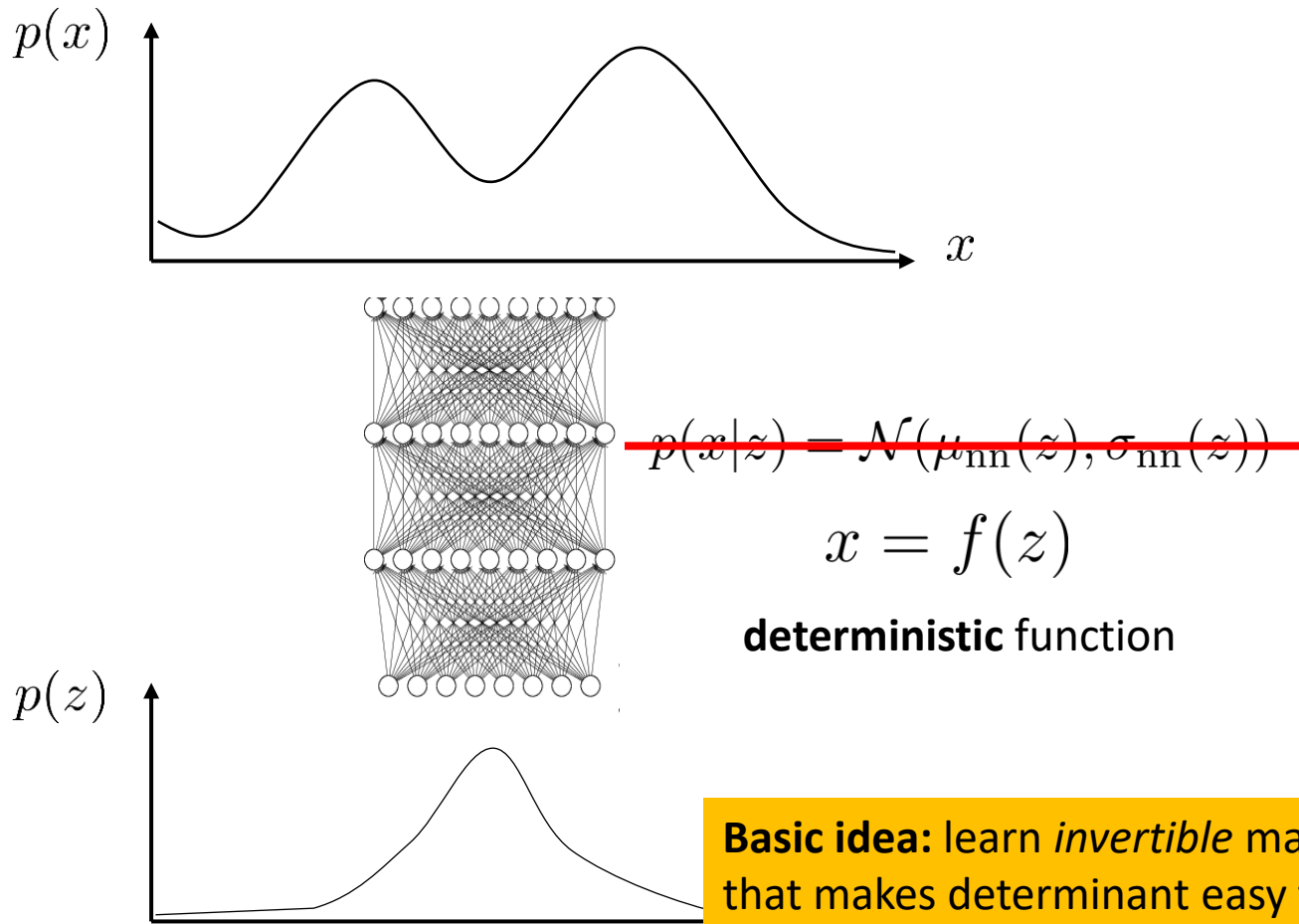
could **schedule**  $\beta$

start low (to get VAE to use  $z$  to reconstruct)

end high (to get samples to be good)

# Invertible Models and Normalizing Flows

# A simpler kind of model



Why is this such a big deal?

change of variables formula:

$$p(x) = p(z) \left| \det \left( \frac{df(z)}{dz} \right) \right|^{-1}$$

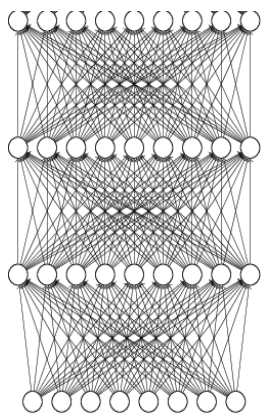
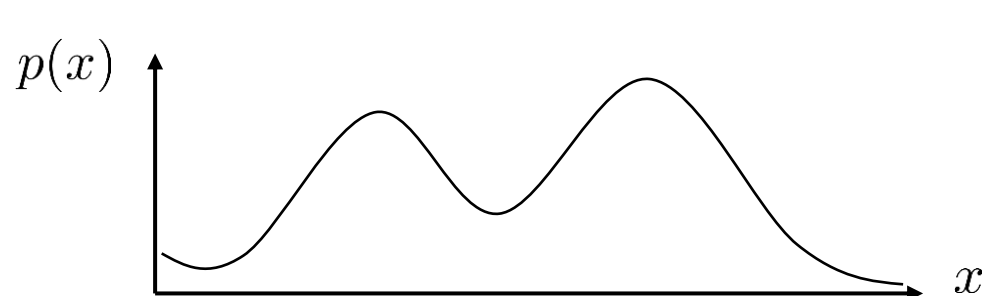
where  $z = f^{-1}(x)$

correction for change in  
local density due to  $f$

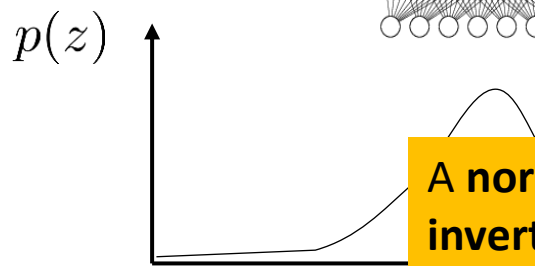
**Basic idea:** learn *invertible* mapping from  $z$  to  $x$   
that makes determinant easy to compute

No more need for lower bounds! Can get exact  
probabilities/likelihoods!

# Normalizing flow models



$$x = f(z)$$



A **normalizing flow** model consists of multiple layers of **invertible transformations**

We need to figure out how to make an invertible layer, and then compose many of them to make a deep network

Training objective:

$$\max_{\theta} \frac{1}{N} \sum_{i=1}^N \log p(x_i)$$



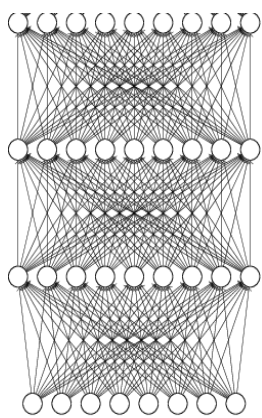
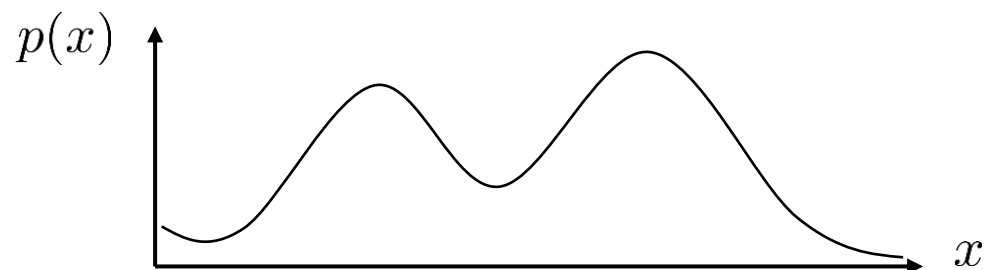
$$\max_{\theta} \frac{1}{N} \sum_{i=1}^N \log p(f^{-1}(x_i)) - \log \left| \det \left( \frac{df(z)}{dz} \right) \right|$$

choose a **special** architecture that makes these easy to compute

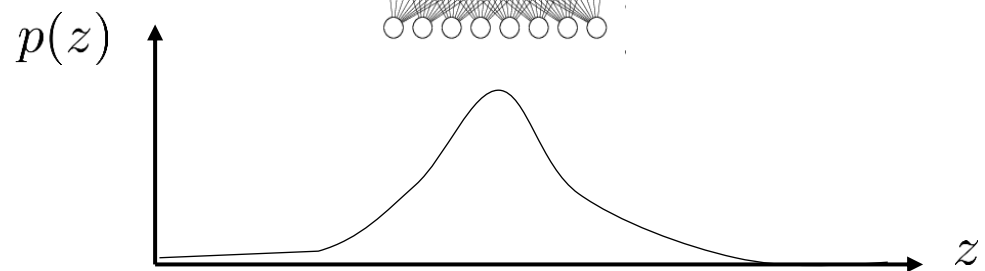
$$p(x) = p(z) \left| \det \left( \frac{df(z)}{dz} \right) \right|^{-1}$$

where  $z = f^{-1}(x)$

# Normalizing flow models



$$x = f(z)$$



$$\max_{\theta} \frac{1}{N} \sum_{i=1}^N \log p(f^{-1}(x_i)) - \log \left| \det \left( \frac{df(z)}{dz} \right) \right|$$

$$f(z) = f_4(f_3(f_2(f_1(z))))$$

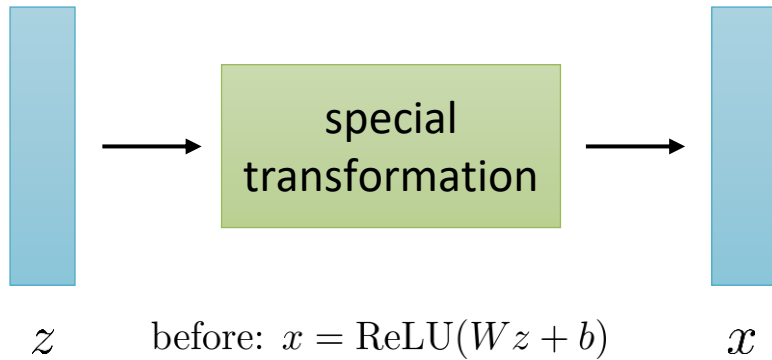
If each **layer** is invertible, the whole thing is invertible

Oftentimes, invertible layers also have very convenient determinants

Log-determinant of whole model is just the sum of log-determinants of the layers

**Goal:** design an invertible layer, and then compose many of them to create a fully invertible neural net

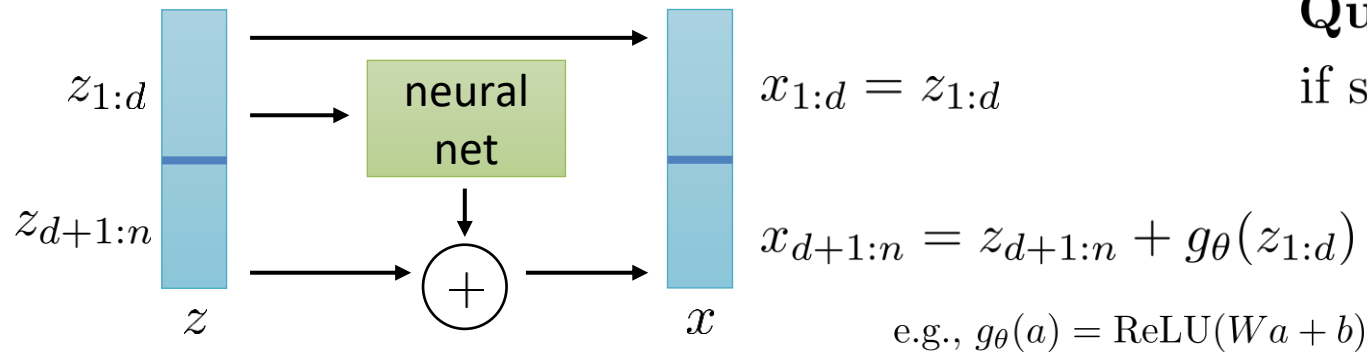
# NICE: Nonlinear Independent Components Estimation



before:  $x = \text{ReLU}(Wz + b)$   
but this is **not** invertible

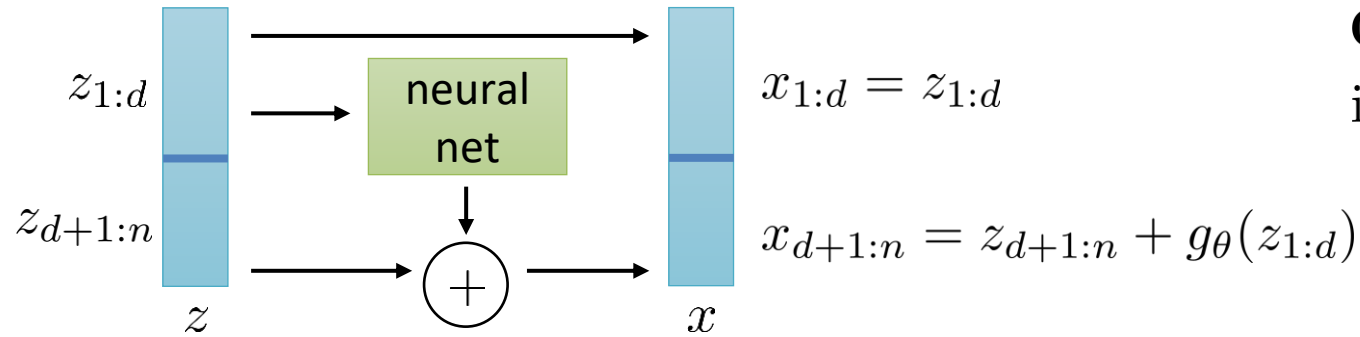
**Idea:** what if we force **part** of the layer to keep all the information so that we can then recover anything that was changed by the nonlinear transformation?

**Important:** here I describe the case for **one** layer, but in reality we'll have many layers!

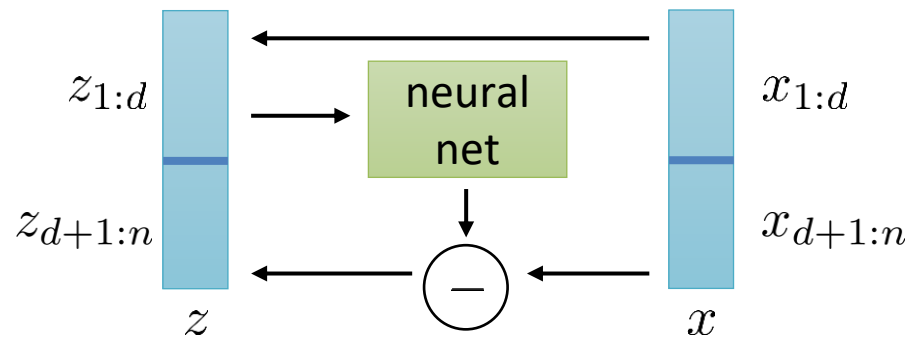


**Question:** if we have  $x$ , can we recover  $z$ ?  
if so, then this layer is **invertible**

# NICE: Nonlinear Independent Components Estimation



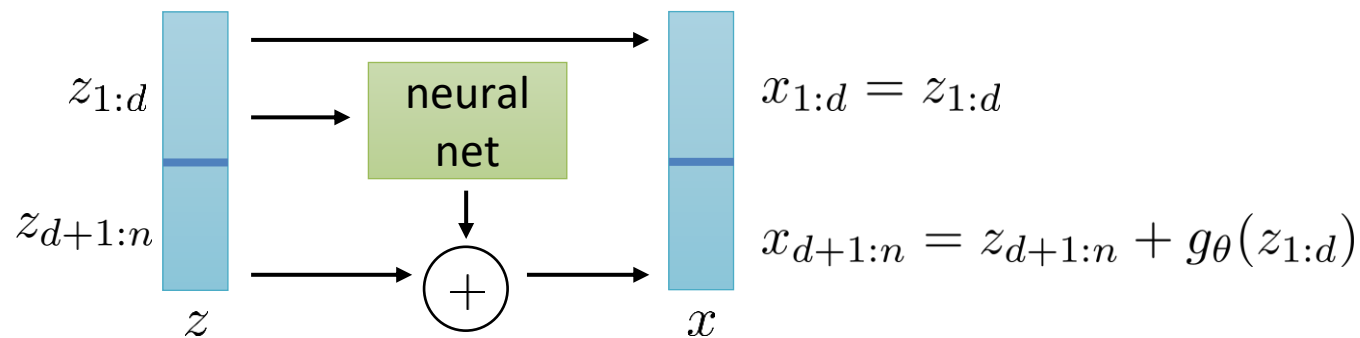
**Question:** if we have  $x$ , can we recover  $z$ ?  
if so, then this layer is **invertible**



1. Recover  $z_{1:d} = x_{1:d}$
2. Recover  $g_{\theta}(z_{1:d})$
3. Recover  $z_{d+1:n} = x_{d+1:n} - g_{\theta}(z_{1:d})$



# What about the Jacobian?



$$\left| \det \left( \frac{df(z)}{dz} \right) \right| = 1$$

This is very simple and convenient

But it's representationally a bit limiting

$$\frac{df(z)}{dz} = \begin{bmatrix} \frac{dx_{1:d}}{dz_{1:d}} & \frac{dx_{1:d}}{dz_{d+1:n}} \\ \frac{dx_{d+1:n}}{dz_{1:d}} & \frac{dx_{d+1:n}}{dz_{d+1:n}} \end{bmatrix} = \begin{bmatrix} \mathbf{I} & 0 \\ \frac{dg_{\theta}}{dz_{1:d}} & \mathbf{I} \end{bmatrix}$$

Arrows indicate the following assignments:

- $\mathbf{I}$  points to  $\frac{dx_{1:d}}{dz_{1:d}}$
- $0$  points to  $\frac{dx_{1:d}}{dz_{d+1:n}}$
- $\frac{dg_{\theta}}{dz_{1:d}}$  points to  $\frac{dx_{d+1:n}}{dz_{1:d}}$
- $\mathbf{I}$  points to  $\frac{dx_{d+1:n}}{dz_{d+1:n}}$

# NICE: Nonlinear Independent Components Estimation



(a) Model trained on MNIST



(b) Model trained on TFD

# NICE: Nonlinear Independent Components Estimation

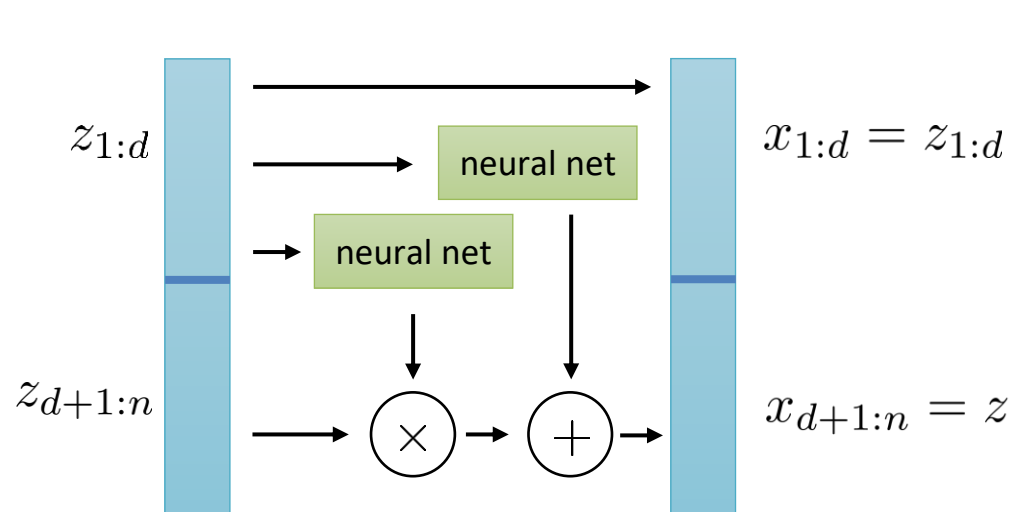


(c) Model trained on SVHN



(d) Model trained on CIFAR-10

# Real-NVP: Non-Volume Preserving Transformation



**Inverse** can be derived in the same way as before:

1. Recover  $z_{1:d} = x_{1:d}$
2. Recover  $g_{\theta}(z_{1:d})$  and  $h_{\theta}(z_{1:d})$
3. Recover  $z_{d+1:n} = (x_{d+1:n} - g_{\theta}(z_{1:d})) / \exp(h_{\theta}(z_{1:d}))$

$$x_{d+1:n} = z_{d+1:n} \times \exp(h_{\theta}(z_{1:d})) + g_{\theta}(z_{1:d})$$

↑  
elementwise product

$$\left| \det \left( \frac{df(z)}{dz} \right) \right| = \prod_{i=d+1}^n \exp(h_{\theta}(z_{1:d})_i)$$

$$\frac{df(z)}{dz} = \begin{bmatrix} \mathbf{I} & 0 \\ \frac{dx_{d+1:n}}{dz_{1:d}} & \text{diag}(\exp(h_{\theta}(z_{1:d}))) \end{bmatrix}$$

This is significantly more expressive



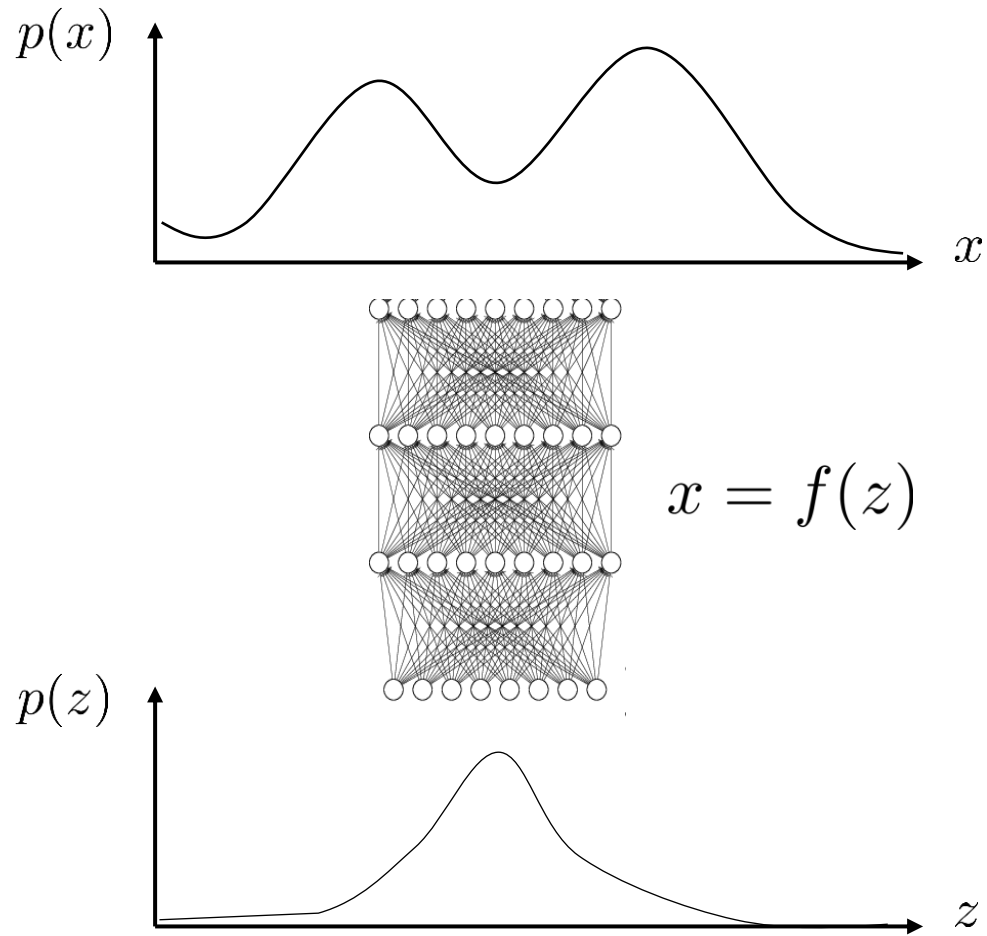
# Real-NVP Samples



Material based on Grover & Ermon CS236

Dinh et al. **Density estimation using Real-NVP**. 2016.

# Concluding Remarks



- + can get exact probabilities/likelihoods
- + no need for lower bounds
- + conceptually simpler (perhaps)
- requires special architecture
- $Z$  must have same dimensionality as  $X$

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