

Latent Variable Models

Designing, Visualizing and Understanding Deep Neural Networks

CS W182/282A

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UC Berkeley

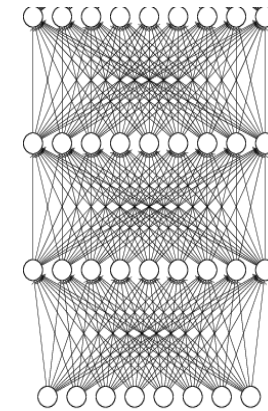
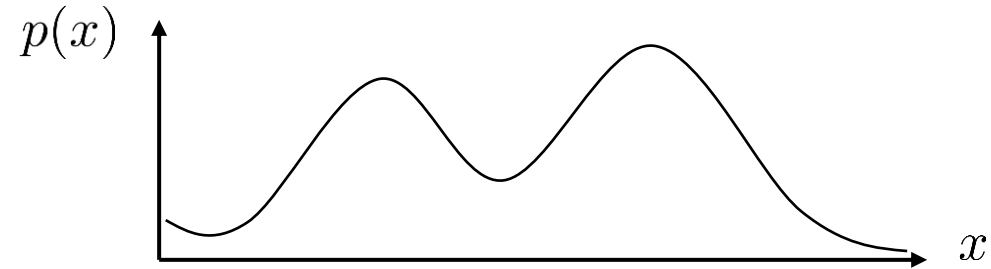


Latent variable models in general

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

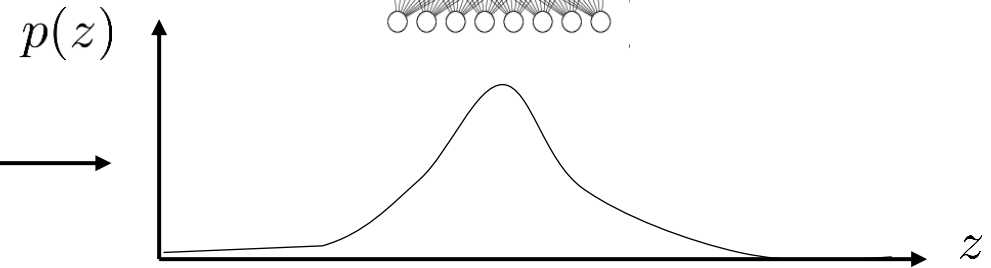
“easy” distribution
(e.g., conditional Gaussian)

“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:

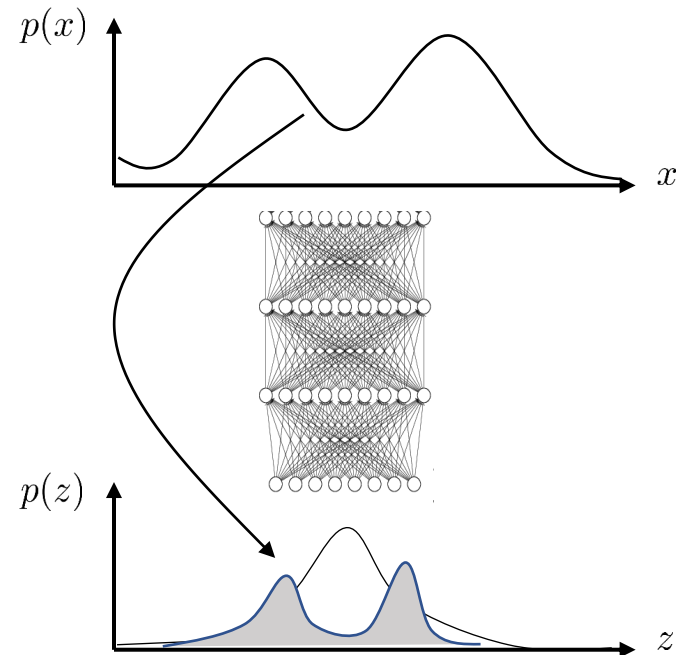
$$\theta \leftarrow \arg \max_{\theta} \frac{1}{N} \sum_i E_{z \sim p(z|x_i)} [\log p_{\theta}(x_i, z)]$$

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 $p(z|x_i)$



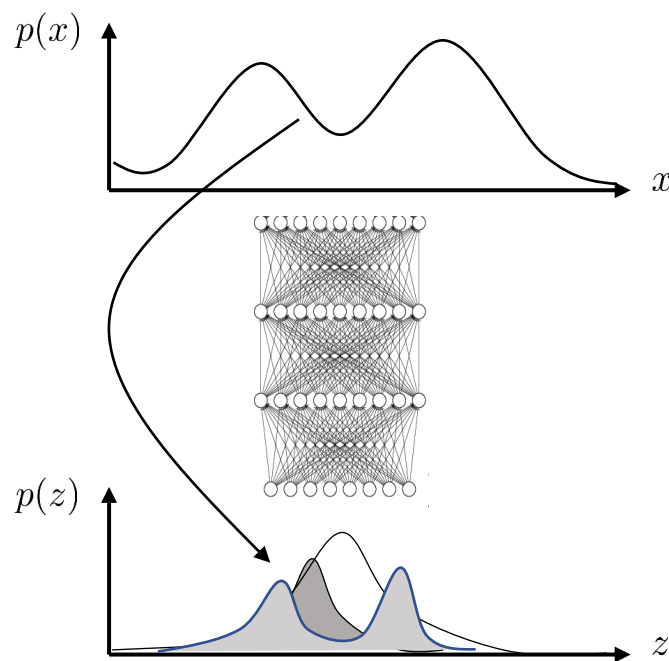
The variational approximation

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:

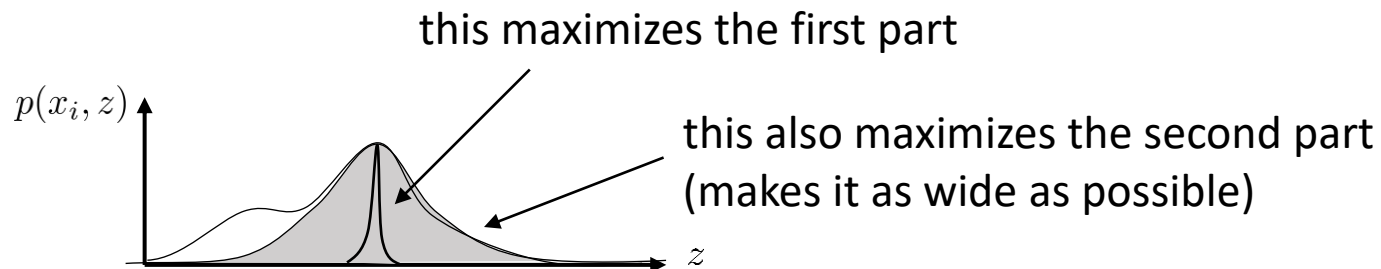
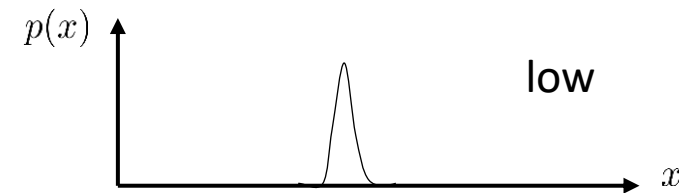
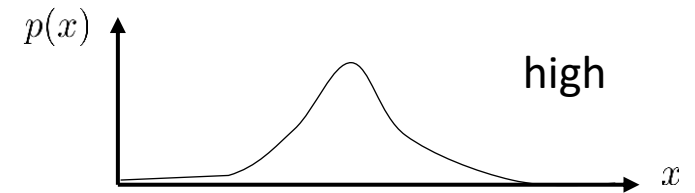
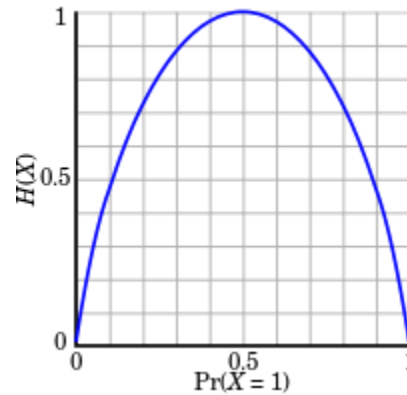
$$\mathcal{H}(p) = -E_{x \sim p(x)}[\log p(x)] = - \int_x p(x) \log p(x) dx$$

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...

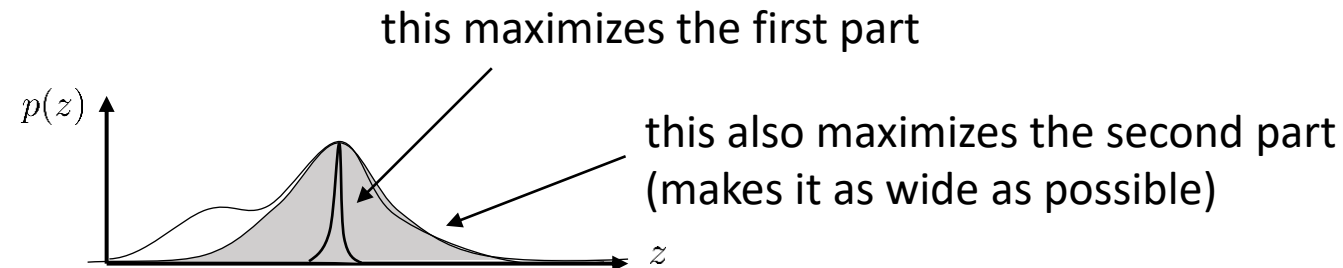
KL-Divergence:

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

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

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

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

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

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

how?

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 μ_i, σ_i

What's the problem?

for each x_i (or mini-batch):

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

sample $z \sim q_i(z)$

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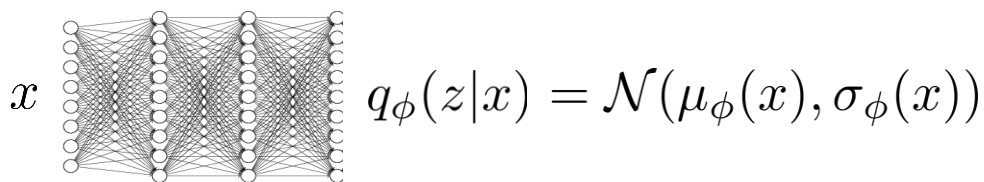
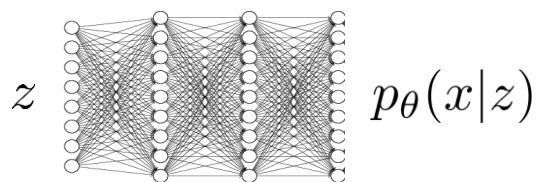
gradient ascent on μ_i, σ_i

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 $\nabla_{\sigma_i} \mathcal{L}_i(p, q_i)$

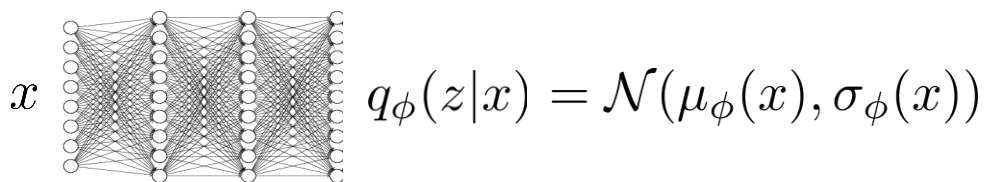
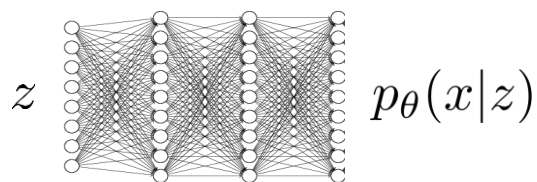
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How many parameters are there?

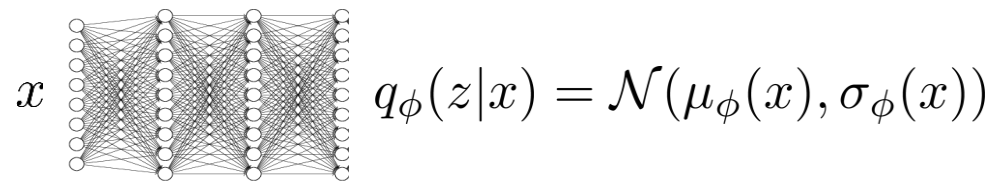
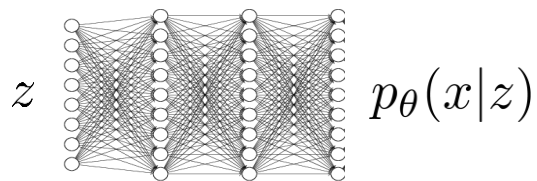
$$|\theta| + (|\mu_i| + |\sigma_i|) \times N$$

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!

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

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

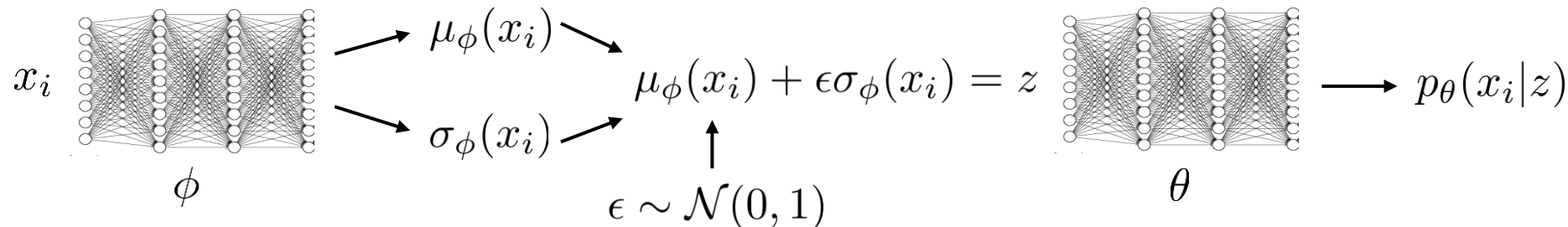


$$\epsilon \sim \mathcal{N}(0, 1)$$

independent of ϕ !

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

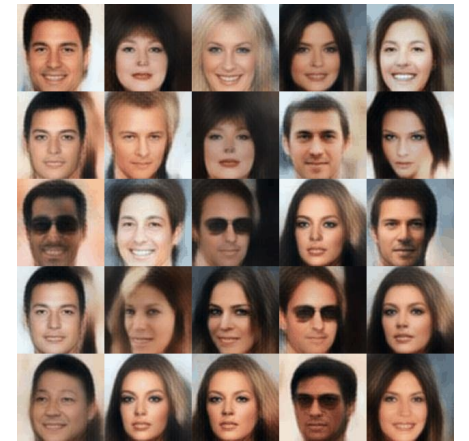
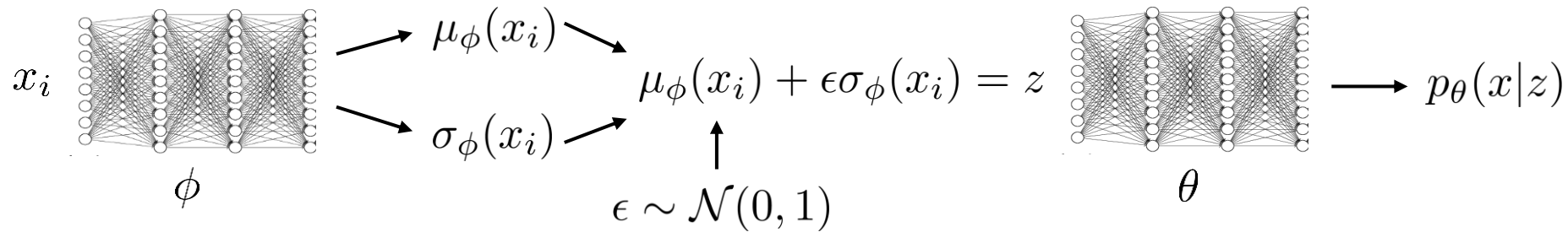
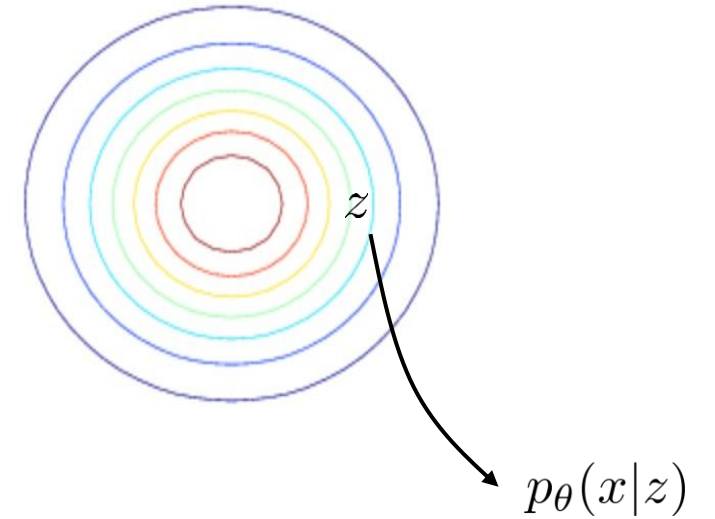
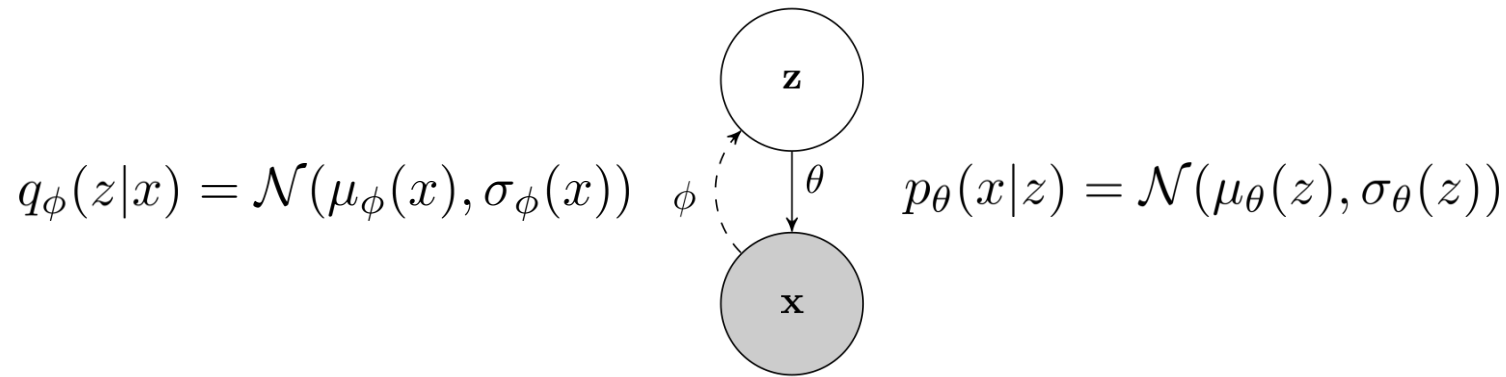
- Policy gradient
 - Can handle both discrete and continuous latent variables
 - High variance, requires multiple samples & small learning rates
- Reparameterization trick
 - Only continuous latent variables
 - Very simple to implement
 - Low variance

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

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

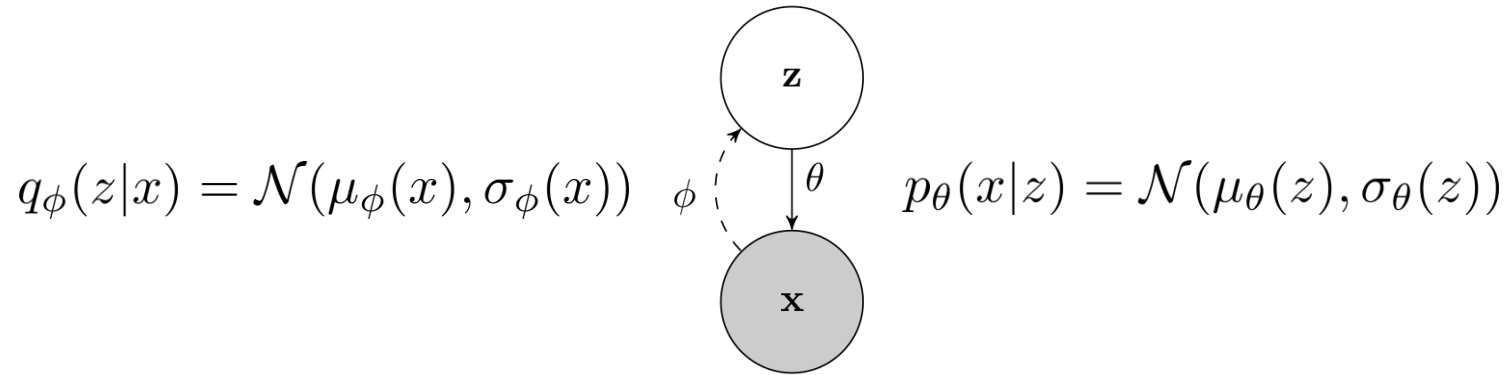
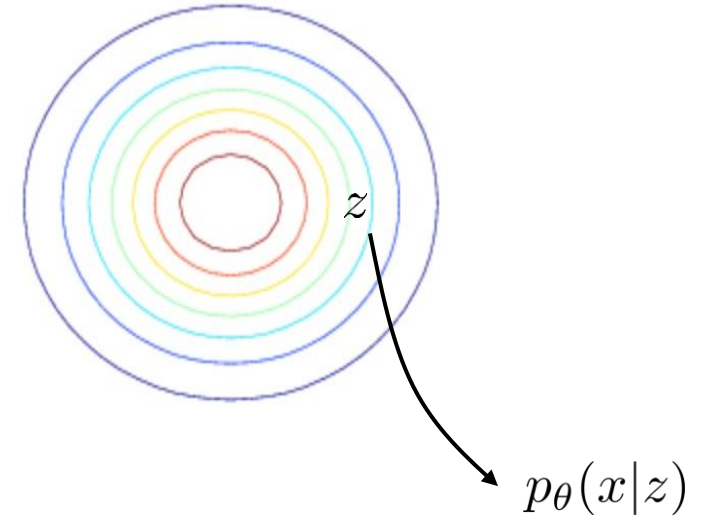
Variational Autoencoders

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



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

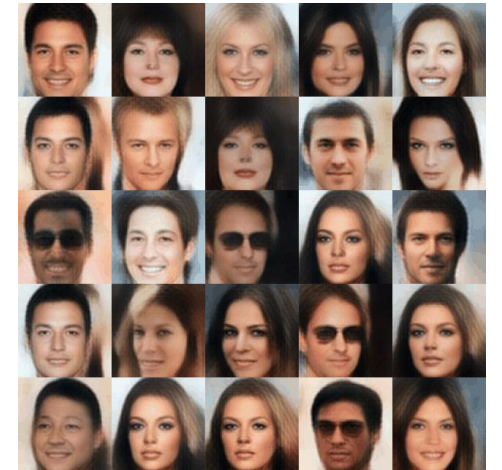
why does this work?

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

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

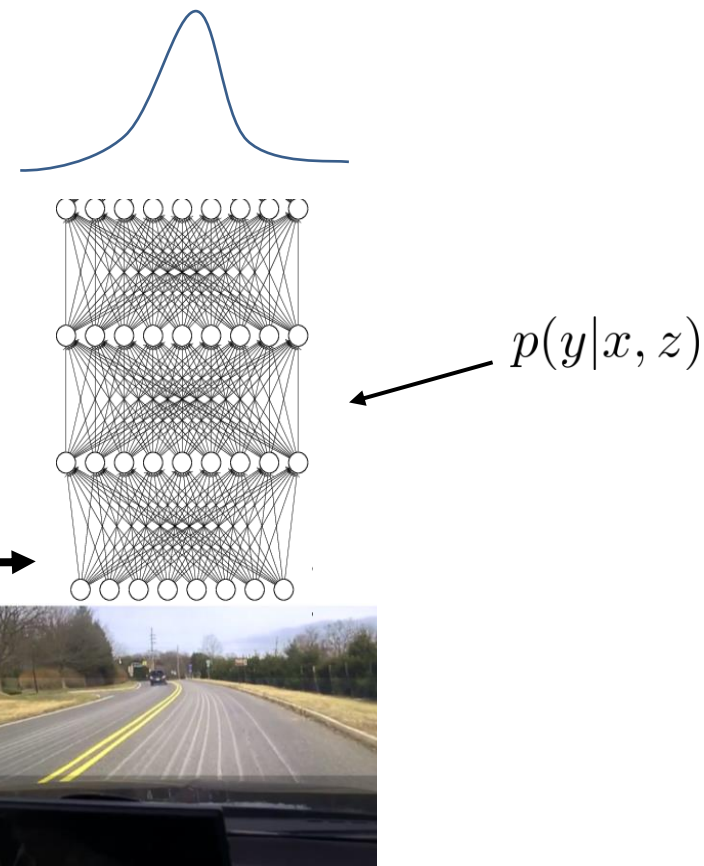
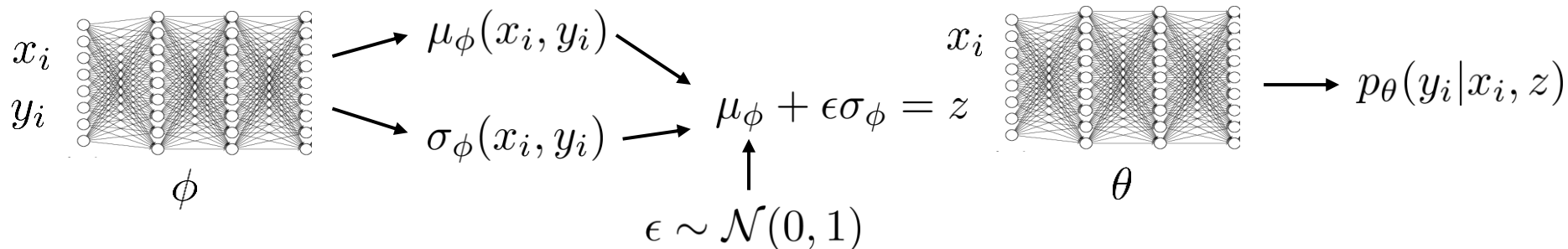
just like before, only now generating y_i
and *everything* is conditioned on x_i

at test time:

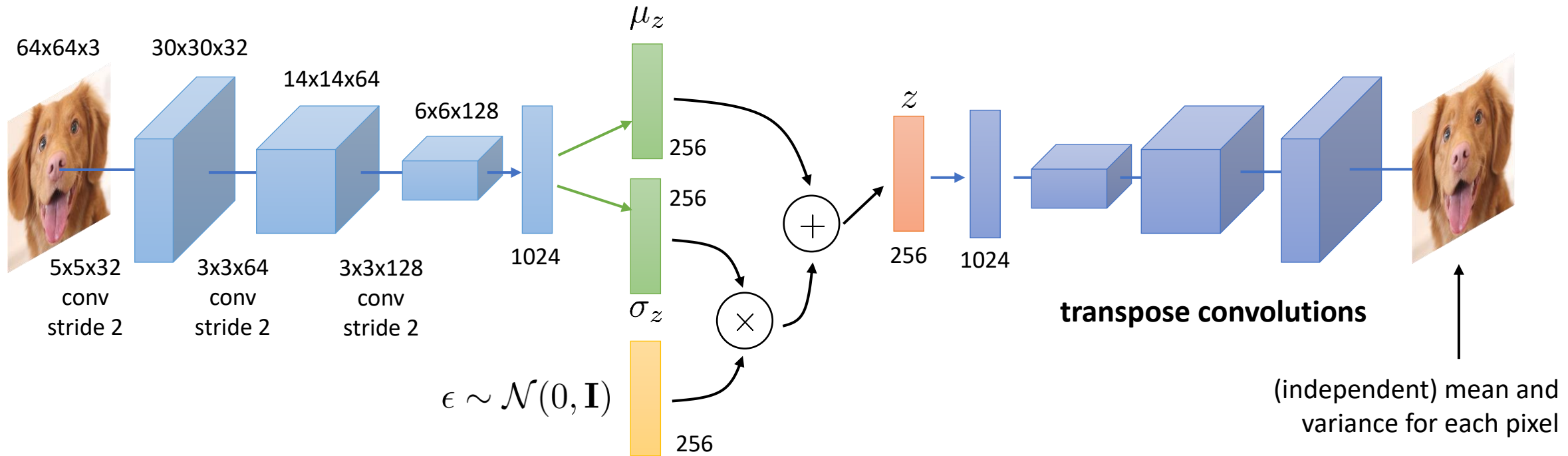
$$z \sim p(z|x_i)$$

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

can *optionally* depend on x



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 β manually to get good reconstructions **and** good samples

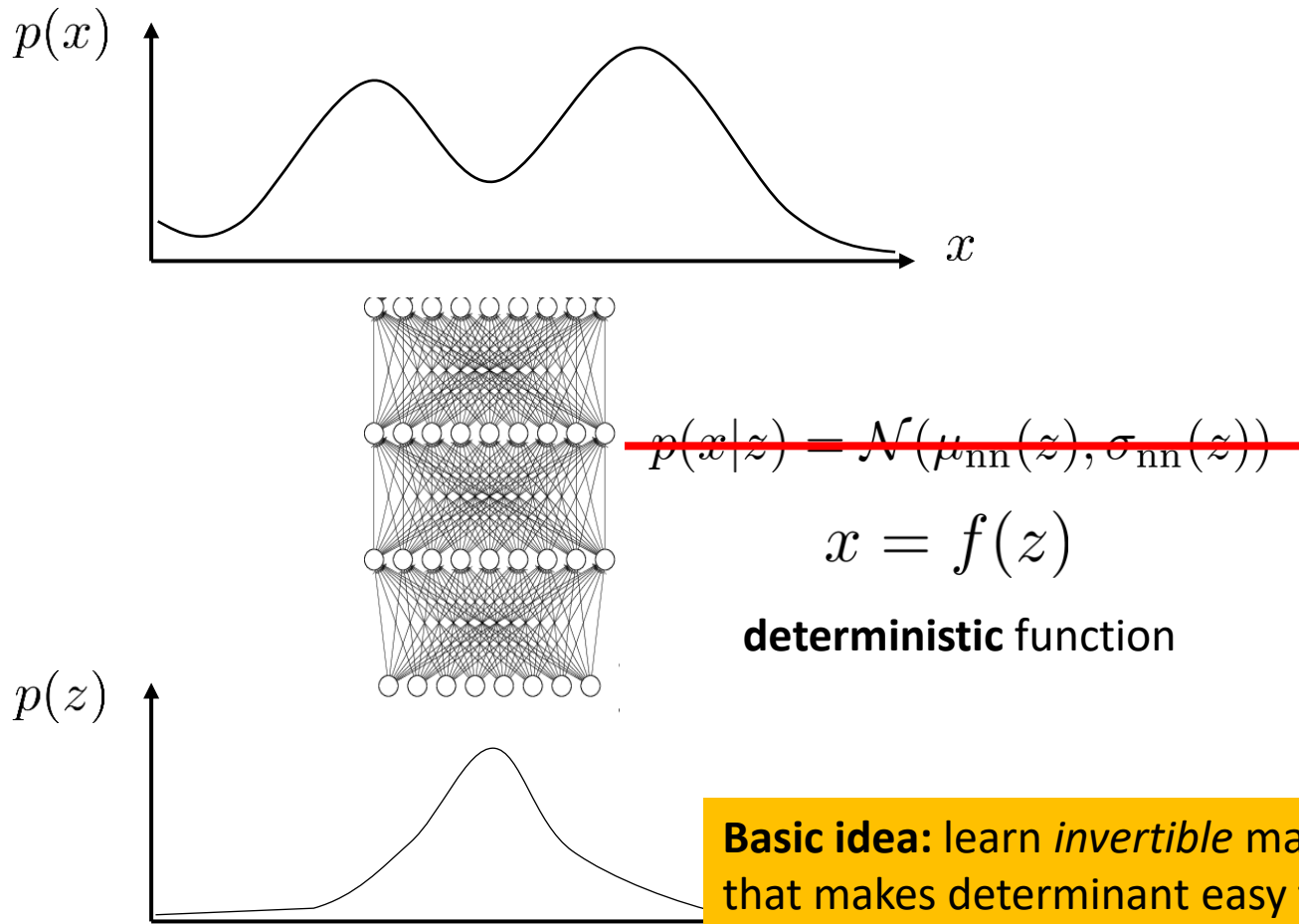
could **schedule** β

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:

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

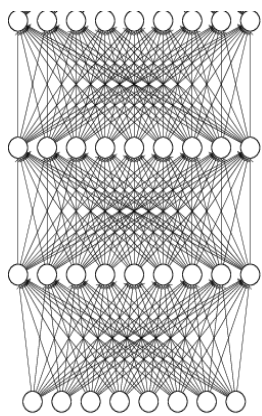
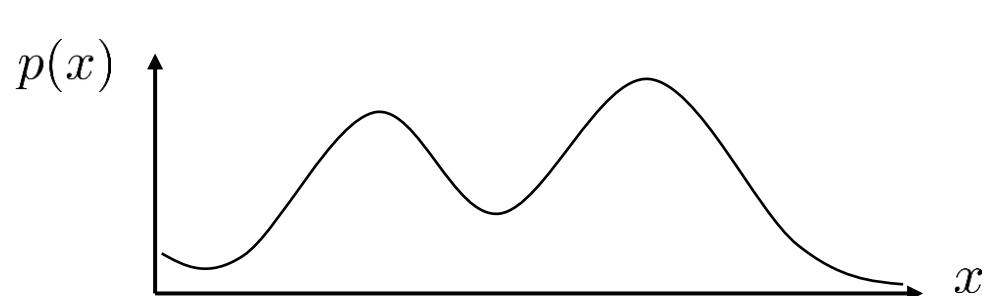
where $z = f^{-1}(x)$

correction for change in
local density due to f

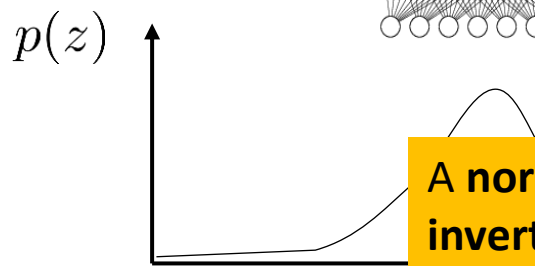
Basic idea: learn *invertible* mapping from z to x
that makes determinant easy to compute

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:

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



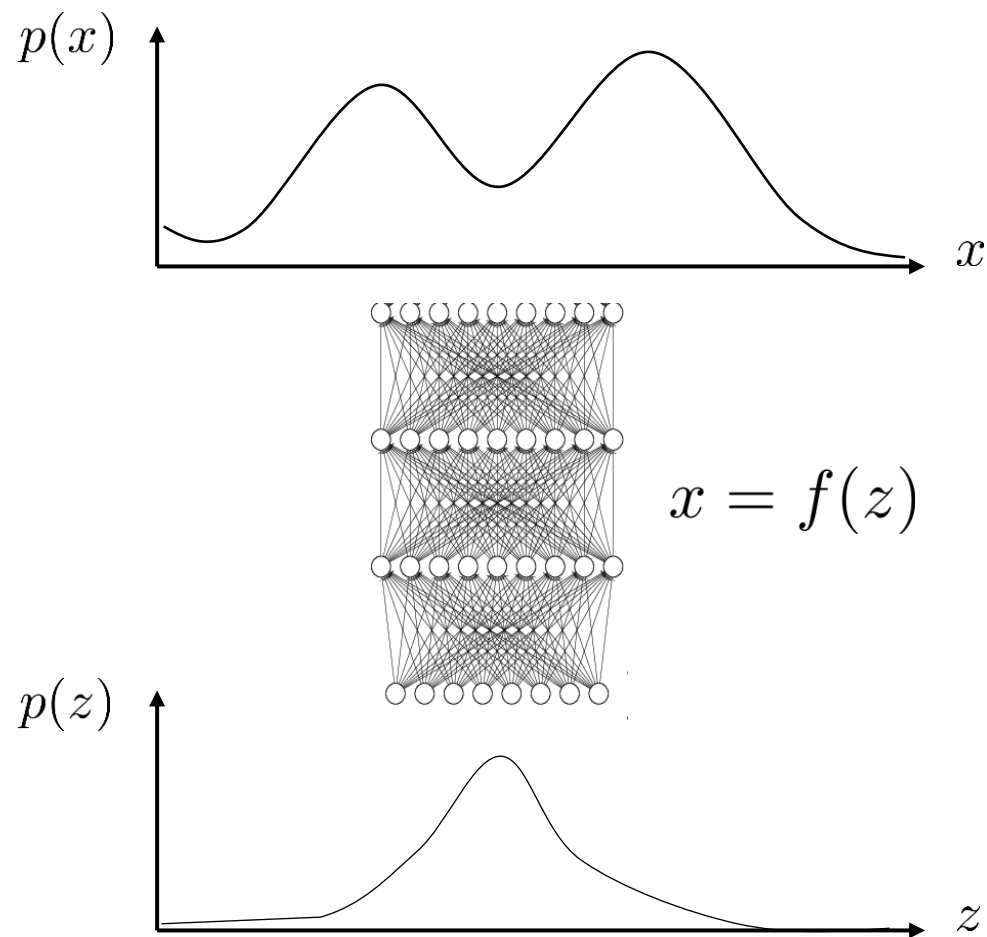
$$\max_{\theta} \frac{1}{N} \sum_{i=1}^N \log p(f^{-1}(x_i)) - \log \left| \det \left(\frac{df(z)}{dz} \right) \right|$$

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



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

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

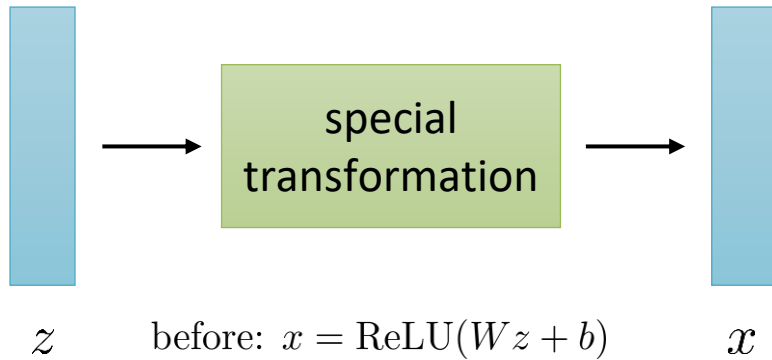
If each **layer** is invertible, the whole thing is invertible

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

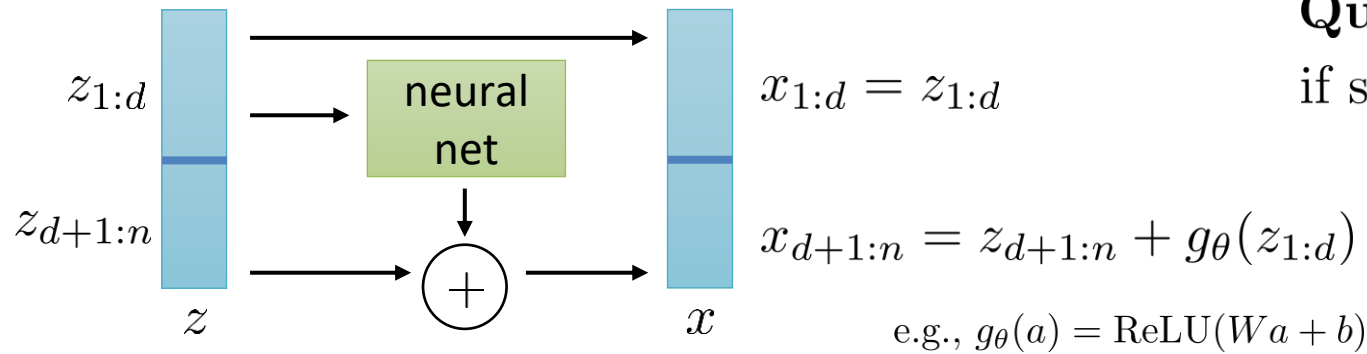
NICE: Nonlinear Independent Components Estimation



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

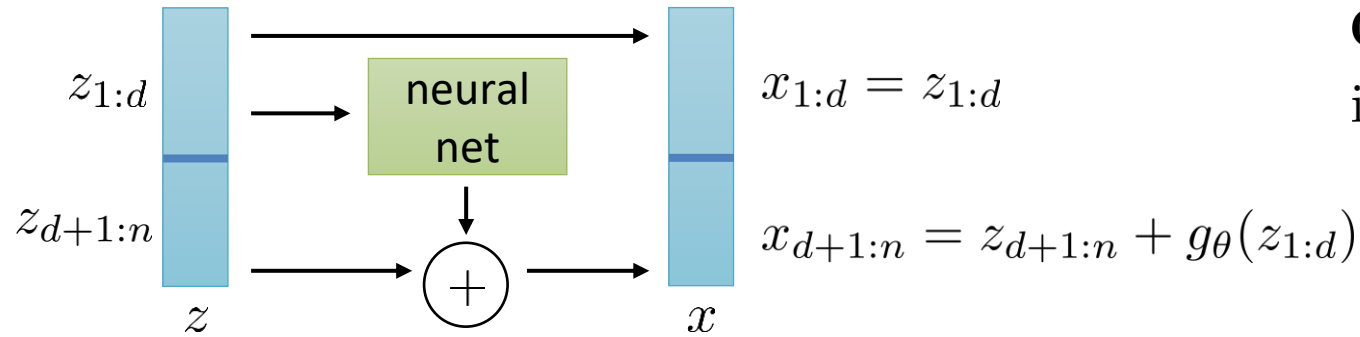
Idea: what if we force **part** of the layer to keep all the information so that we can then recover anything that was changed by the nonlinear transformation?

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

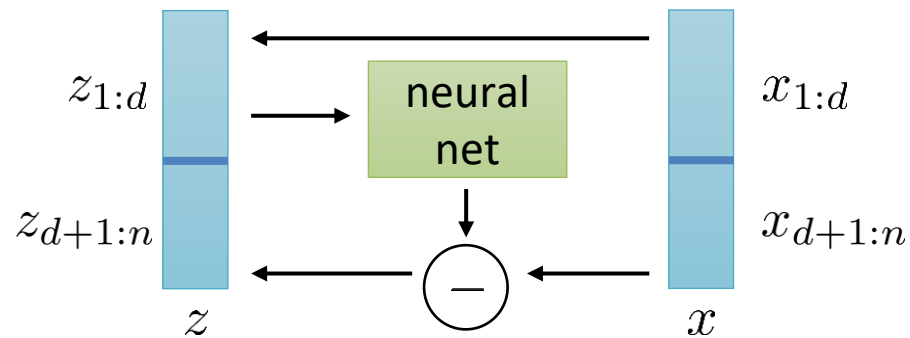


Question: if we have x , can we recover z ?
if so, then this layer is **invertible**

NICE: Nonlinear Independent Components Estimation

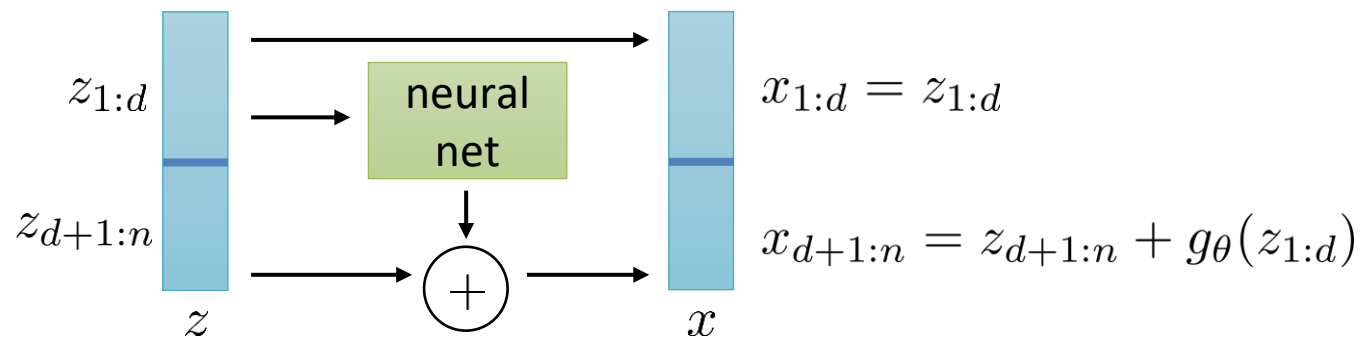


Question: if we have x , can we recover z ?
if so, then this layer is **invertible**



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

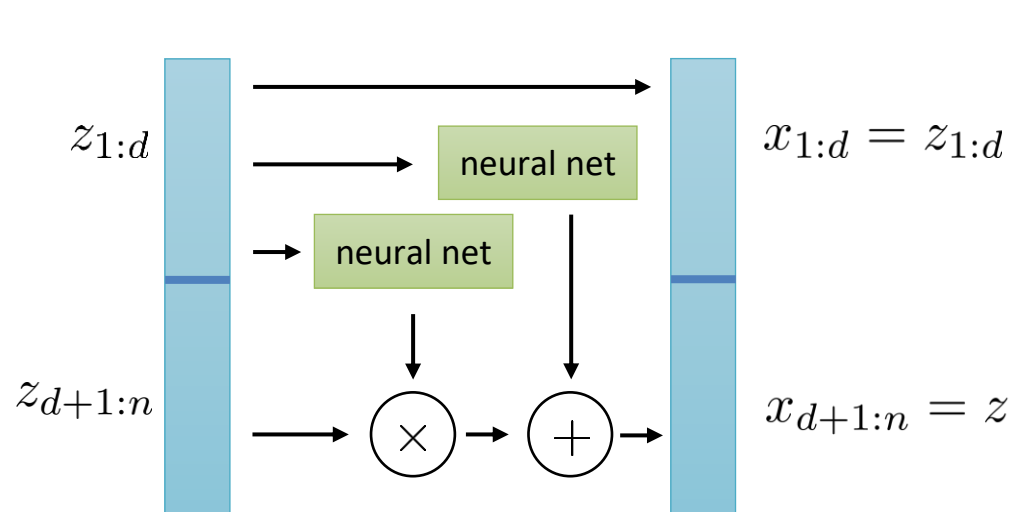


(c) Model trained on SVHN



(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

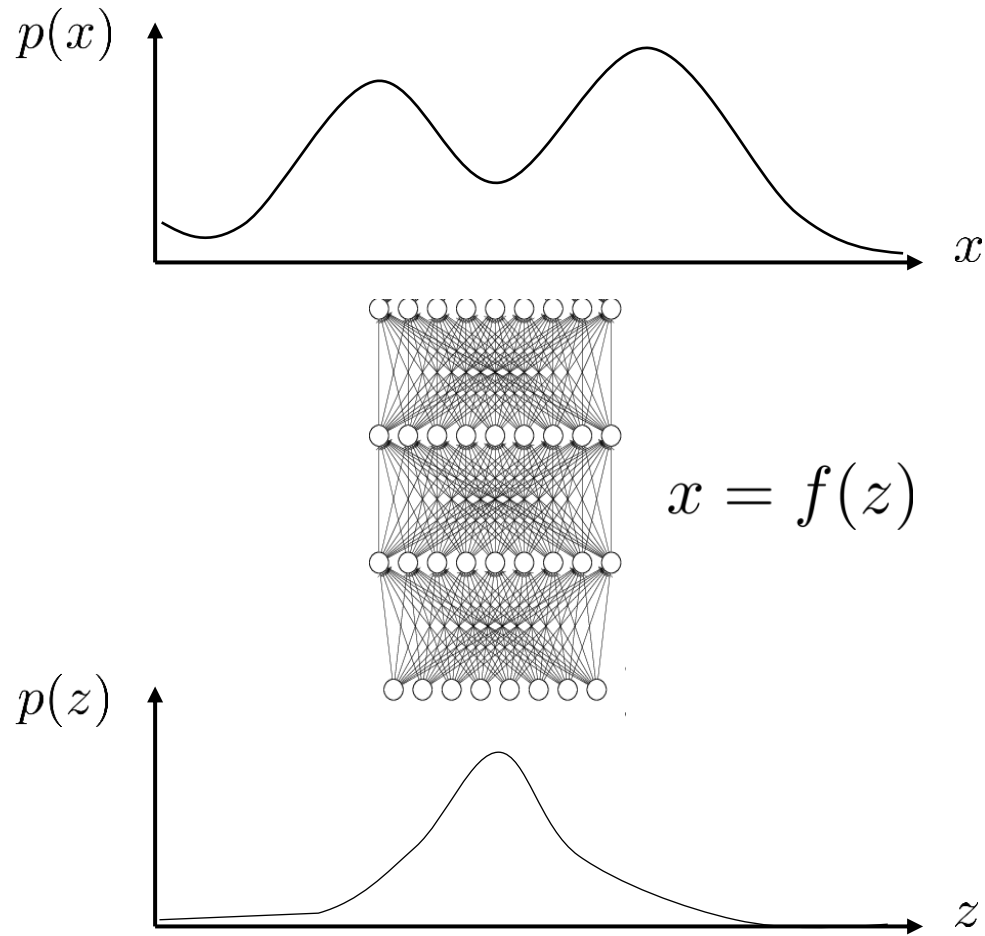
Real-NVP Samples



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