CSC421/2516 Lecture 15: Reversible and Autoregressive Models

Roger Grosse and Jimmy Ba

Overview

- In generative modeling, we'd like to train a network that models a distribution, such as a distribution over images.
- One way to judge the quality of the model is to sample from it.
- This field has seen rapid progress:

2009

2015

2018

Overview

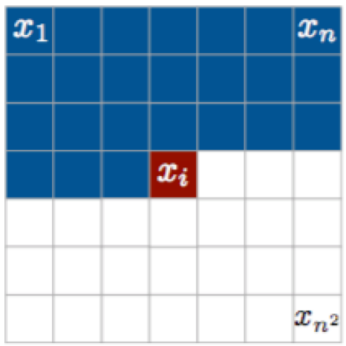
Four modern approaches to generative modeling:

- Autoregressive models (Lectures 5 and 13, this lecture, next lecture)
- Reversible architectures (this lecture)
- Variational autoencoders (Lecture 17)
- Generative adversarial networks (Lecture 19)

All four approaches have different pros and cons.

Autoregressive Models

- We've already looked at autoregressive models in this course:
  - Neural language models
  - RNN language models (and decoders)
- We can push this further, and generate very long sequences.



Treat an image as a very long sequence using raster scan order

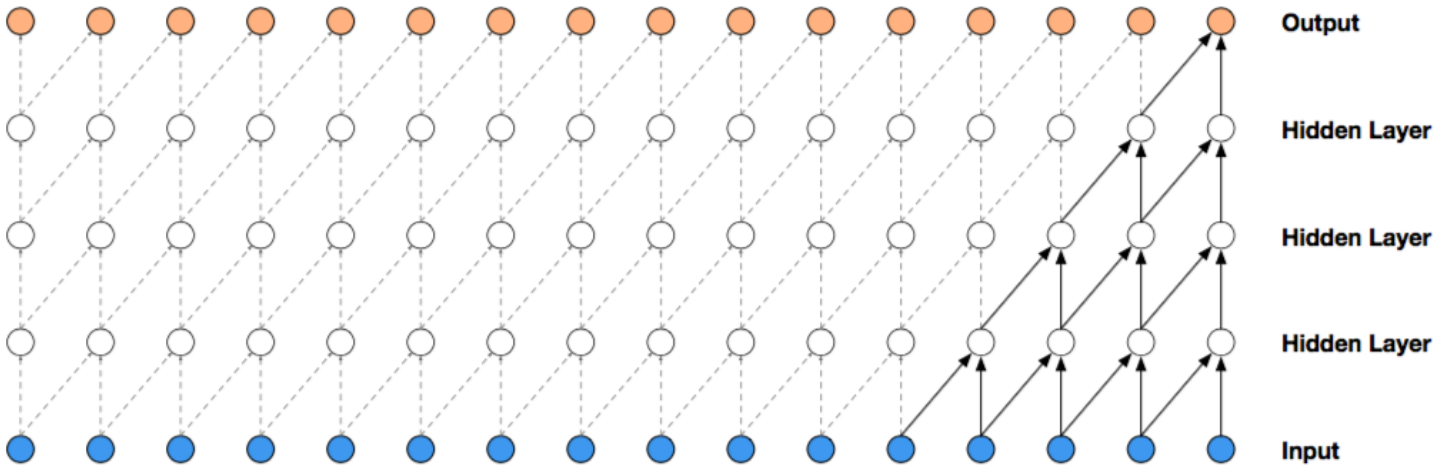
A speech signal can be represented as a waveform, with at least 16,000 samples per second.

- Problem: training an RNN to generate these sequences requires a for loop over $>$ 10,000 time steps.

Causal Convolution

Idea 1: causal convolution

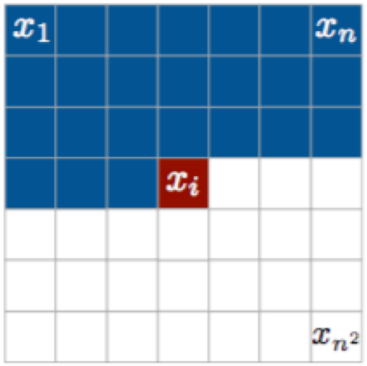
- For RNN language models, we used the training sequence as both the inputs and the outputs to the RNN.
  - We made sure the model was causal: each prediction depended only on inputs earlier in the sequence.
- We can do the same thing using a convolutional architecture.



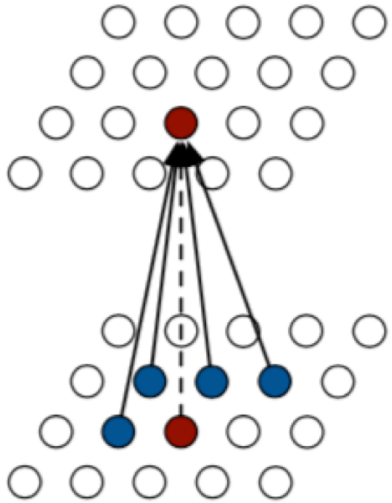
- No for loops! Processing each input sequence just requires a series of convolution operations.

Causal Convolution

Causal convolution for images:

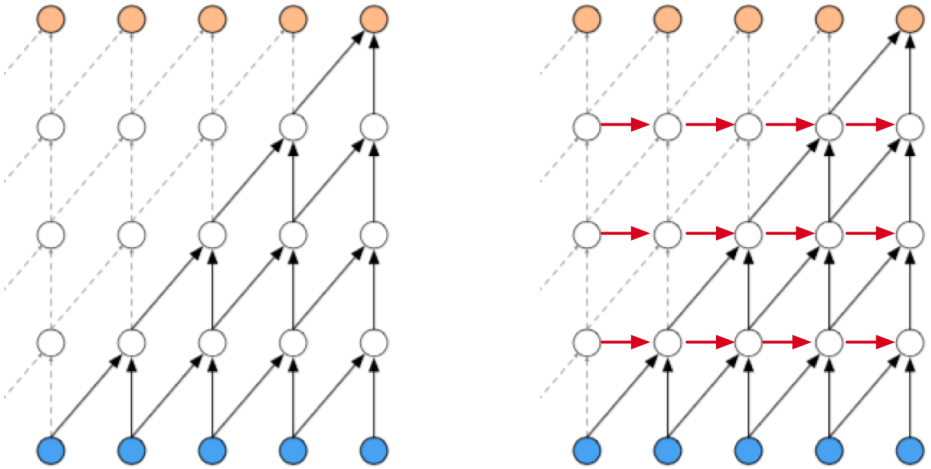


The image is treated as a very long sequence of pixels using raster scan order.



We can restrict the connectivity pattern in each layer to make it causal. This can be implemented by clamping some weights to zero.

CNN vs. RNN



- We can turn a causal CNN into an RNN by adding recurrent connections. Is this a good idea?
  - The RNN has a memory, so it can use information from all past time steps. The CNN has a limited context.
  - But training the RNN is very expensive since it requires a for loop over time steps. The CNN only requires a series of convolutions.
  - Generating from both models is very expensive, since it requires a for loop. (Whereas generating from a GAN or a reversible model is very fast.)

PixelCNN and PixelRNN

- Van den Oord et al., ICML 2016, "Pixel recurrent neural networks"
- This paper introduced two autoregressive models of images: the PixelRNN and the PixelCNN. Both generated amazingly good high-resolution images.
- The output is a softmax over 256 possible pixel intensities.
- Completing an image using an PixelCNN:

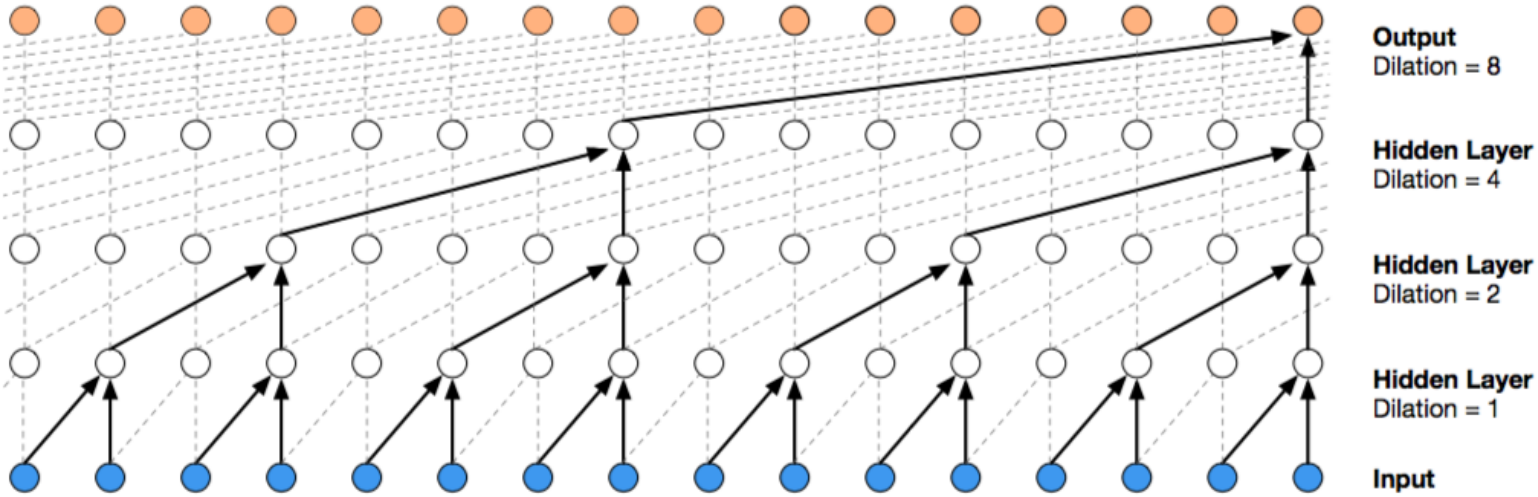
PixelCNN and PixelRNN

Samples from a PixelRNN trained on ImageNet:

Dilated Convolution

Idea 2: dilated convolution

- The advantage of RNNs over CNNs is that their memory lets them learn arbitrary long-distance dependencies.
- But we can dramatically increase a CNN's receptive field using dilated convolution.



WaveNet

- WaveNet is an autoregressive model for raw audio based on causal dilated convolutions.
  - van den Oord et al., 2016. "WaveNet: a generative model for raw audio".
- Audio needs to be sampled at at least 16k frames per second for good quality. So the sequences are very long.
- WaveNet uses dilations of $1, 2, \ldots, 512$, so each unit at the end of this block as a receptive field of length 1024, or 64 milliseconds.
- It stacks several of these blocks, so the total context length is about 300 milliseconds.
- `https://deepmind.com/blog/wavenet-generative-model-raw-audio/`

Overview

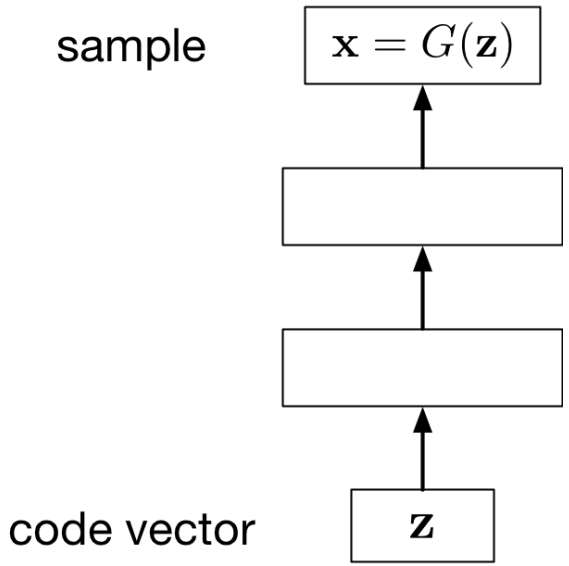
Four modern approaches to generative modeling:

- Autoregressive models (Lectures 5 and 13, this lecture, next lecture)
- Reversible architectures (this lecture)
- Variational autoencoders (Lecture 17)
- Generative adversarial networks (Lecture 19)

All four approaches have different pros and cons.

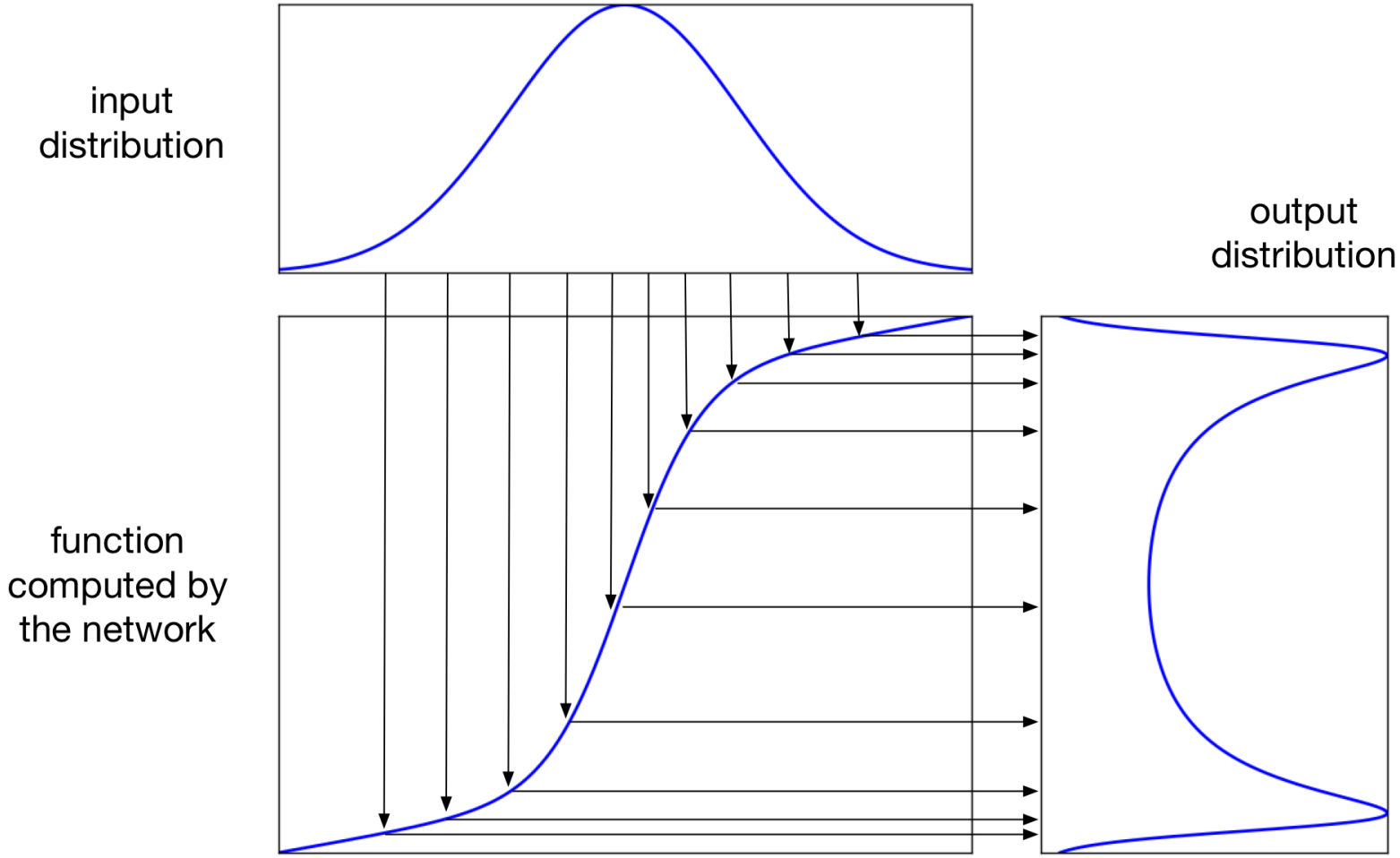
Generator Networks

- Autoregressive models explicitly predict a distribution at each step.
- Another approach to generative modeling is to train a neural net to produce approximate samples from the distribution.
- Start by sampling the code vector $\mathbf{z}$ from a fixed, simple distribution (e.g. spherical Gaussian)
- The generator network computes a differentiable function G mapping $\mathbf{z}$ to an $\mathbf{x}$ in data space

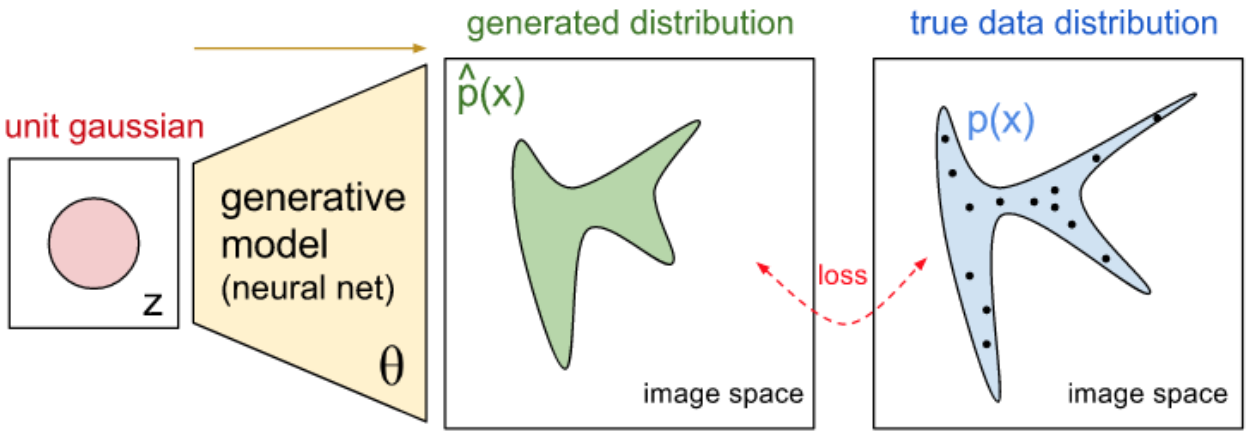


Generator Networks

A 1-dimensional example:

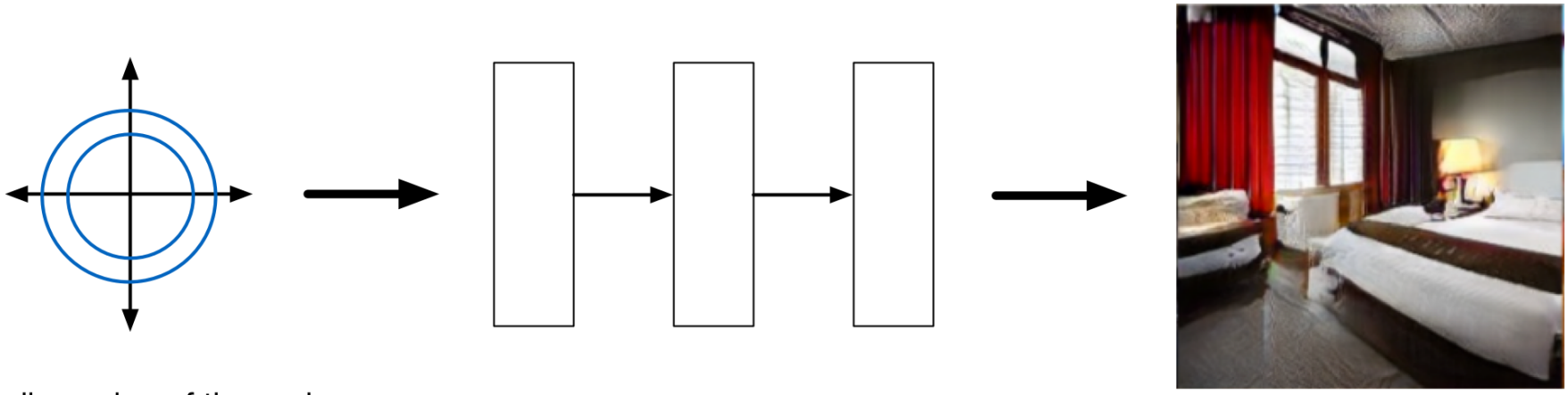


Generator Networks



https://blog.openai.com/generative-models/

Generator Networks



Each dimension of the code vector is sampled independently from a simple distribution, e.g. Gaussian or uniform.

This is fed to a (deterministic) generator network.

The network outputs an image.

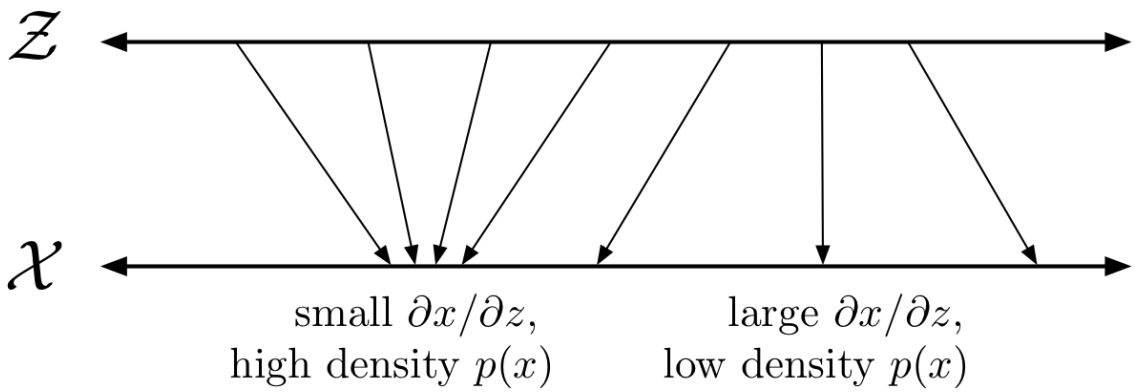
This sort of architecture sounded preposterous to many of us, but amazingly, it works.

Change of Variables Formula

- Let f denote a differentiable, bijective mapping from space $\mathcal{Z}$ to space $\mathcal{X}$. (I.e., it must be 1-to-1 and cover all of $\mathcal{X}$.)
- Since f defines a one-to-one correspondence between values $\mathbf{z} \in \mathcal{Z}$ and $\mathbf{x} \in \mathcal{X}$, we can think of it as a change-of-variables transformation.
- Change-of-Variables Formula from probability theory: if $\mathbf{x} = f(\mathbf{z})$, then

$$p_X(\mathbf{x}) = p_Z(z) \left| \det \left(\frac{\partial \mathbf{x}}{\partial \mathbf{z}} \right) \right|^{-1}$$

- Intuition for the Jacobian term:



Change of Variables Formula

- Suppose we have a generator network which computes the function f. It's tempting to apply the change-of-variables formula in order to compute the density $p_X(\mathbf{x})$.
- I.e., compute $\mathbf{z} = f^{-1}(\mathbf{x})$

$$p_X(\mathbf{x}) = p_Z(z) \left| \det \left(\frac{\partial \mathbf{x}}{\partial z} \right) \right|^{-1}$$

- Problems?

Change of Variables Formula

- Suppose we have a generator network which computes the function f. It's tempting to apply the change-of-variables formula in order to compute the density $p_X(\mathbf{x})$.
- I.e., compute $\mathbf{z} = f^{-1}(\mathbf{x})$

$$p_X(\mathbf{x}) = p_Z(z) \left| \det \left(\frac{\partial \mathbf{x}}{\partial z} \right) \right|^{-1}$$

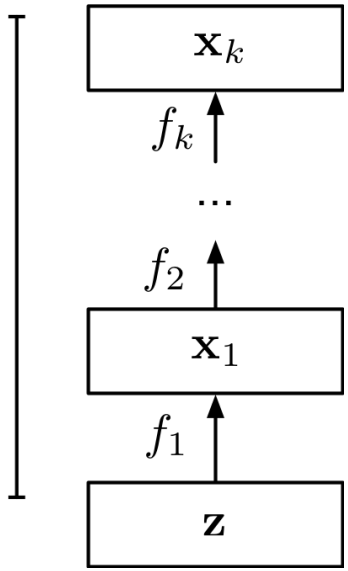
- Problems?
  - It needs to be differentiable, so that the Jaobian $\partial \mathbf{x} / \partial z$ is defined.
  - The mapping f needs to be invertible, with an easy-to-compute inverse.
  - We need to be able to compute the (log) determinant.
- Differentiability is easy (just use a differentiable activation function), but the other requirements are trickier.

Reversible Blocks

- Now let's define a reversible block which is invertible and has a tractable determinant.

- Such blocks can be composed.
  - Inversion: $f^{-1} = f_1^{-1} \circ \cdots \circ f_k^{-1}$
  - Determinants: $\left|\frac{\partial \mathbf{x}_k}{\partial \mathbf{z}}\right| = \left|\frac{\partial \mathbf{x}_k}{\partial \mathbf{x}_{k-1}}\right| \cdots \left|\frac{\partial \mathbf{x}_2}{\partial \mathbf{x}_1}\right| \left|\frac{\partial \mathbf{x}_1}{\partial \mathbf{z}}\right|$

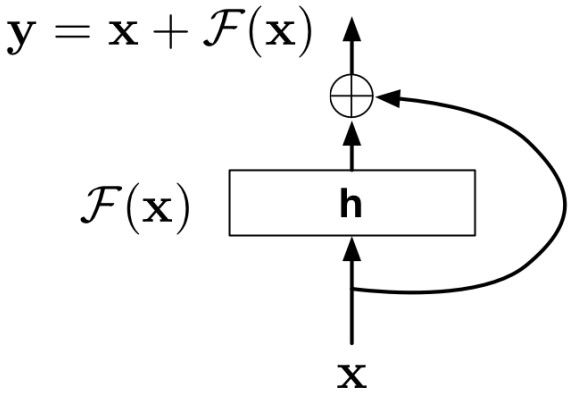
$$f = f_k \circ \cdots \circ f_1$$



Reversible Blocks

- Recall the residual blocks:

$$\mathbf{y} = \mathbf{x} + \mathcal{F}(\mathbf{x})$$

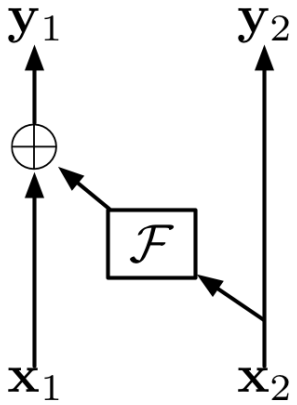


- Reversible blocks are a variant of residual blocks. Divide the units into two groups, $\mathbf{x}_1$ and $\mathbf{x}_2$.

$$\mathbf{y}_1 = \mathbf{x}_1 + \mathcal{F}(\mathbf{x}_2)$$
$$\mathbf{y}_2 = \mathbf{x}_2$$

- Inverting a reversible block:

$$\mathbf{x}_2 = \mathbf{y}_2$$
$$\mathbf{x}_1 = \mathbf{y}_1 - \mathcal{F}(\mathbf{x}_2)$$



Reversible Blocks

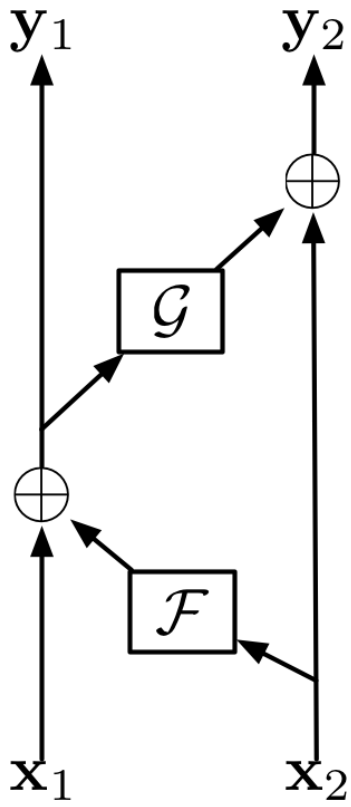
Composition of two reversible blocks, but with $\mathbf{x}_1$ and $\mathbf{x}_2$ swapped:

- Forward:

$$\mathbf{y}_1 = \mathbf{x}_1 + \mathcal{F}(\mathbf{x}_2)$$
$$\mathbf{y}_2 = \mathbf{x}_2 + \mathcal{G}(\mathbf{y}_1)$$

- Backward:

$$\mathbf{x}_2 = \mathbf{y}_2 - \mathcal{G}(\mathbf{y}_1)$$
$$\mathbf{x}_1 = \mathbf{y}_1 - \mathcal{F}(\mathbf{x}_2)$$

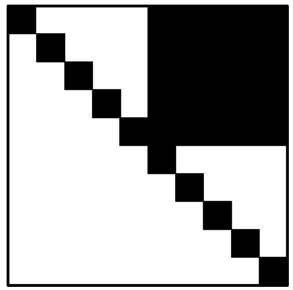


Volume Preservation

- It remains to compute the log determinant of the Jacobian.
- The Jacobian of the reversible block:

$$\mathbf{y}_1 = \mathbf{x}_1 + \mathcal{F}(\mathbf{x}_2)$$
$$\mathbf{y}_2 = \mathbf{x}_2$$

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{pmatrix} \mathbf{I} & \frac{\partial \mathcal{F}}{\partial \mathbf{x}_2} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}$$



- This is an upper triangular matrix. The determinant of an upper triangular matrix is the product of the diagonal entries, or in this case, 1.
- Since the determinant is 1, the mapping is said to be volume preserving.

Nonlinear Independent Components Estimation

- We've just defined the reversible block.
  - Easy to invert by subtracting rather than adding the residual function.
  - The determinant of the Jacobian is 1.
- Nonlinear Independent Components Estimation (NICE) trains a generator network which is a composition of lots of reversible blocks.
- We can compute the likelihood function using the change-of-variables formula:

$$p_X(\mathbf{x}) = p_Z(\mathbf{z}) \left| \det \left(\frac{\partial \mathbf{x}}{\partial \mathbf{z}} \right) \right|^{-1} = p_Z(\mathbf{z})$$

- We can train this model using maximum likelihood. I.e., given a dataset $\{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(N)}\}$, we maximize the likelihood

$$\prod_{i=1}^{N} p_X(\mathbf{x}^{(i)}) = \prod_{i=1}^{N} p_Z(f^{-1}(\mathbf{x}^{(i)}))$$

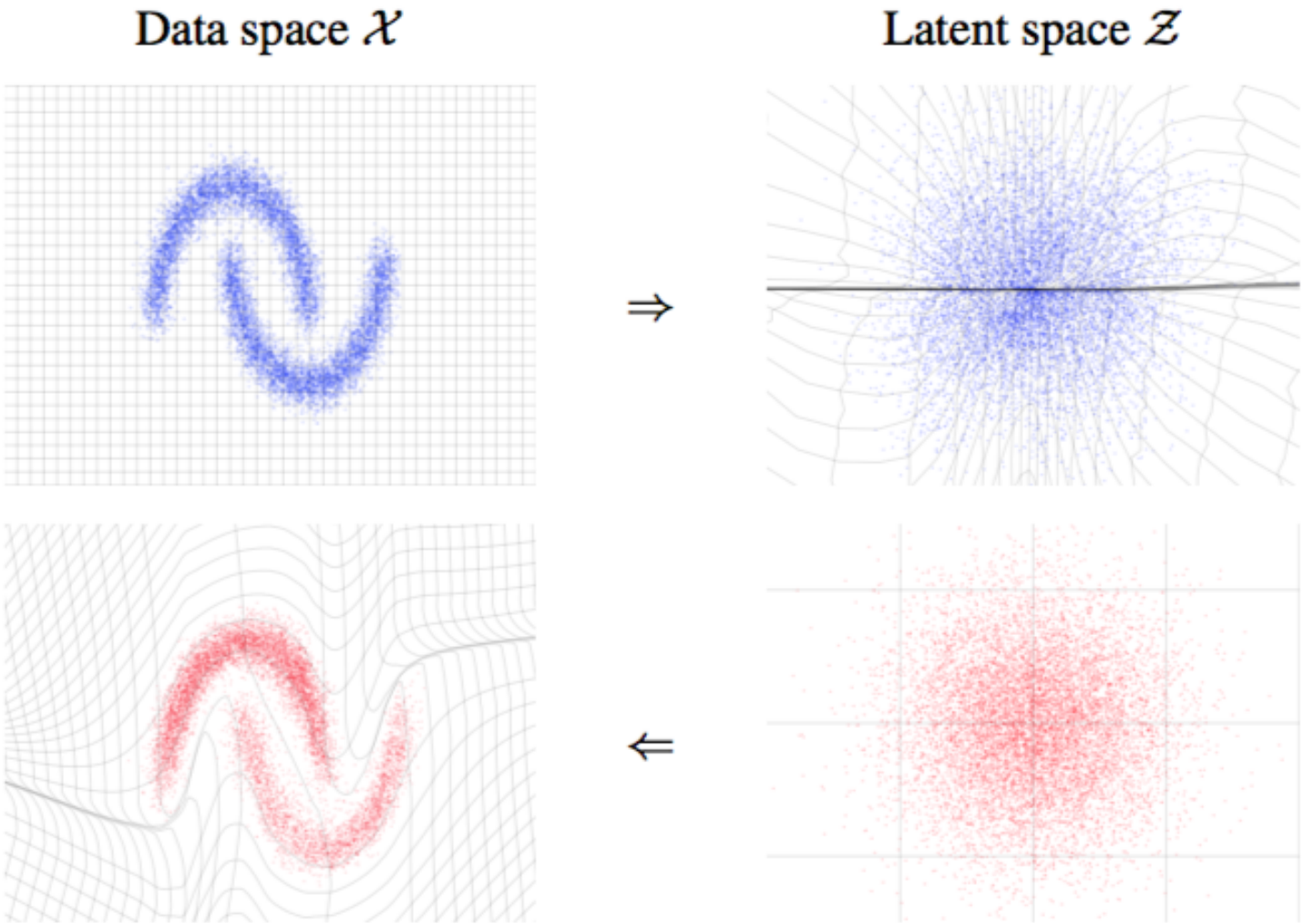
Nonlinear Independent Components Estimation

- Likelihood:

$$p_X(\mathbf{x}) = p_Z(\mathbf{z}) = p_Z(f^{-1}(\mathbf{x}))$$

- Remember, p_Z is a simple, fixed distribution (e.g. independent Gaussians)
- Intuition: train the network such that f^{-1} maps each data point to a high-density region of the code vector space $\mathcal{Z}$.
  - Without constraints on f, it could map everything to $\mathbf{0}$, and this likelihood objective would make no sense.
  - But it can't do this because it's volume preserving.

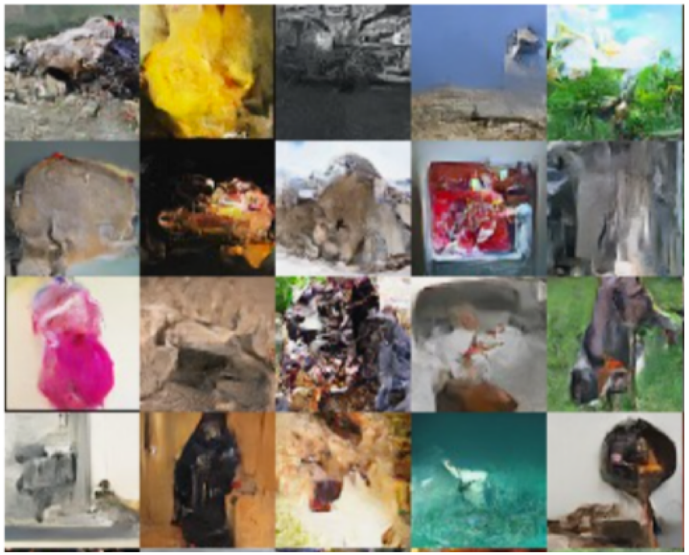
Nonlinear Independent Components Estimation



Dinh et al., 2016. Density estimation using RealNVP.

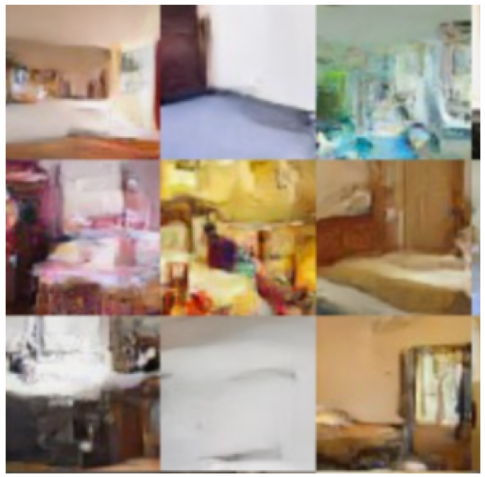
Nonlinear Independent Components Estimation

Samples produced by RealNVP, a model based on NICE.



ImageNet

celebrities



bedrooms

Dinh et al., 2016. Density estimation using RealNVP.

RevNets (optional)

- A side benefit of reversible blocks: you don't need to store the activations in memory to do backprop, since you can reverse the computation.
  - I.e., compute the activations as you need them, moving backwards through the computation graph.
- Notice that reversible blocks look a lot like residual blocks.
- We recently designed a reversible residual network (RevNet) architecture which is like a ResNet, but with reversible blocks instead of residual blocks.
  - Matches state-of-the-art performance on ImageNet, but without the memory cost of activations!
  - Gomez et al., NIPS 2017. "The revesible residual network: backrpop without storing activations".