Generative Modeling

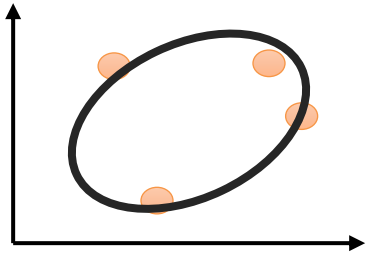
Designing, Visualizing and Understanding Deep Neural Networks

CS W182/282A

Instructor: Sergey Levine
UC Berkeley

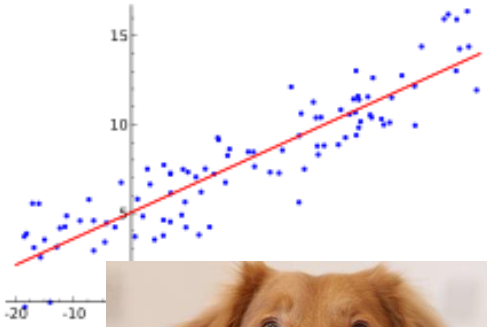
Probabilistic models

$p(x)$



Why would we want to do this?

$p(y|x)$



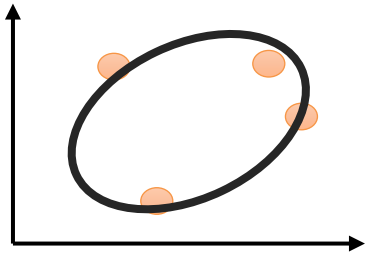
$f_\theta(x) = y$

[object label]

Generative models

$p(x)$

$\mathcal{N}(\mu, \sigma)$

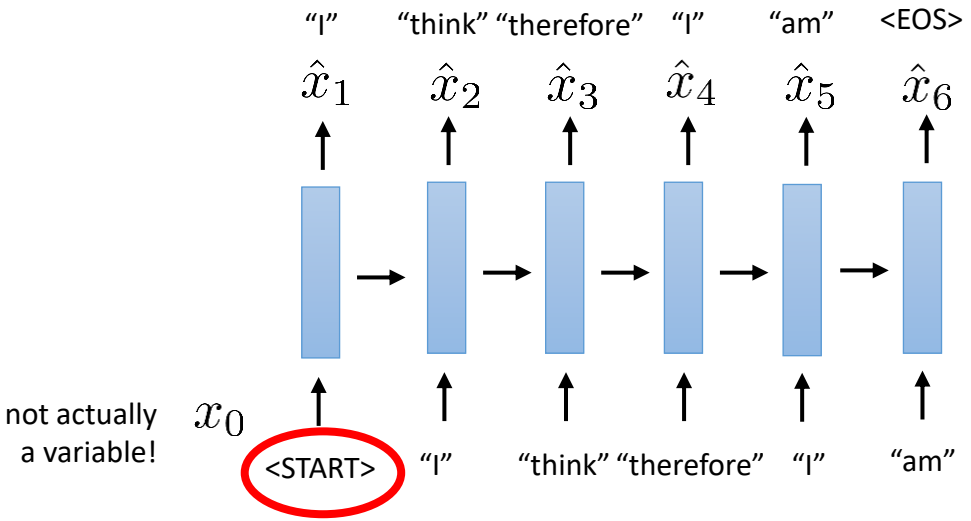


Just different ways to solve the same problem!

Today: can we go from "language models" to "everything models"?

This is called **unsupervised learning**

$$p(x) = p(x_1)p(x_2|x_1)p(x_3|x_{1:2})p(x_4|x_{1:3})p(x_5|x_{1:4})p(x_6|x_{1:5})p(x_{0:5})$$

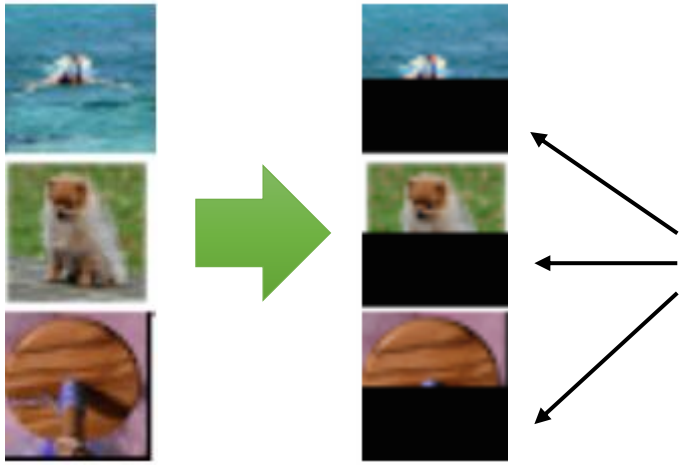


Why would we want to do this?

Same reasons as language modeling!

- Unsupervised pretraining on lots of data
- Representation learning
- Pretraining for later finetuning
- Actually generating things!

Can we “language model” images?

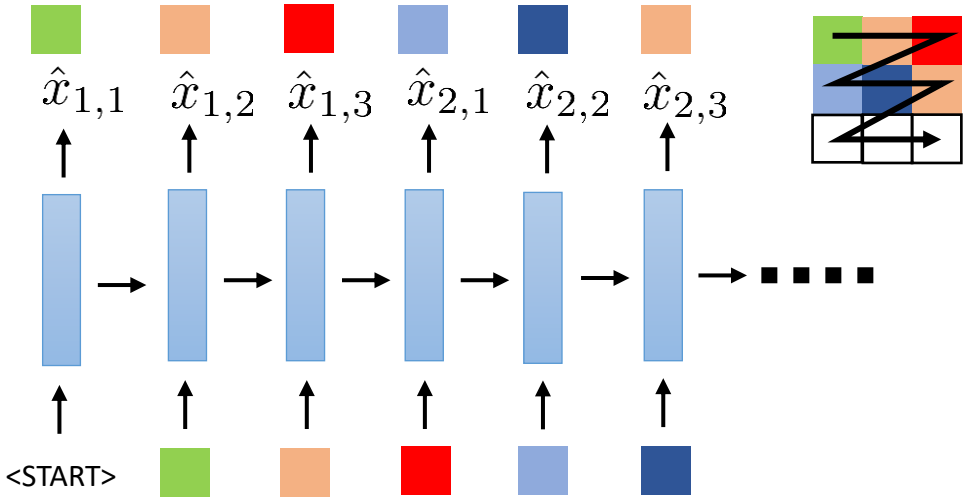


ask the “image language model” to fill in the blanks

before	**now**
time step = word	time step = pixel

some (arbitrary) ordering on pixels

$$p(x) = p(x_1)p(x_2|x_1)p(x_3|x_{1:2})p(x_4|x_{1:3})p(x_5|x_{1:4})p(x_6|x_{1:5})$$



This is basically the main idea, but there are some details we need to figure out!

- How to order the pixels?
- What kind of model to use?

Van den Oord et al. **Pixel Recurrent Neural Networks**. 2016.

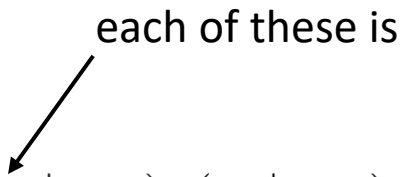
Autoregressive generative models

Main principle for training:

1. Divide up x into dimensions $x_1, \ldots, x_n$
2. Discretize each x_i into k values
3. Model $p(x)$ via the chain rule

   $$p(x) = p(x_1)p(x_2|x_1)p(x_3|x_{1:2})p(x_4|x_{1:3})p(x_5|x_{1:4})p(x_6|x_{1:5})$$

4. Use your favorite sequence model to model $p(x)$



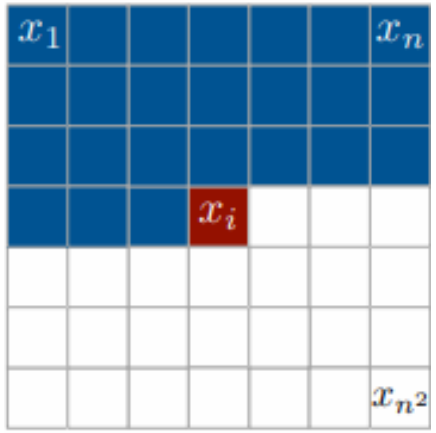
Using autoregressive generative models:

Sampling: ancestral sampling in sequence (x_1, then x_2, etc.)

Completion: feed in actual values for known x_i values

Representations: same idea as ELMo or BERT

PixelRNN



Pixels generated one at a time, left-to-right, top-to-bottom:

$$p(\mathbf{x}) = \prod_{i=1}^{n^2} p(x_i | x_1, ..., x_{i-1})$$

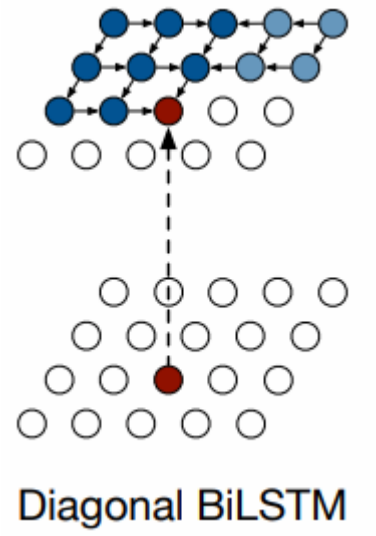
Generate one color channel at a time:

$$p(x_{i,R}|\mathbf{x}_{<i})p(x_{i,G}|\mathbf{x}_{<i}, x_{i,R})p(x_{i,B}|\mathbf{x}_{<i}, x_{i,R}, x_{i,G})$$

256-way softmax

Some practical considerations:

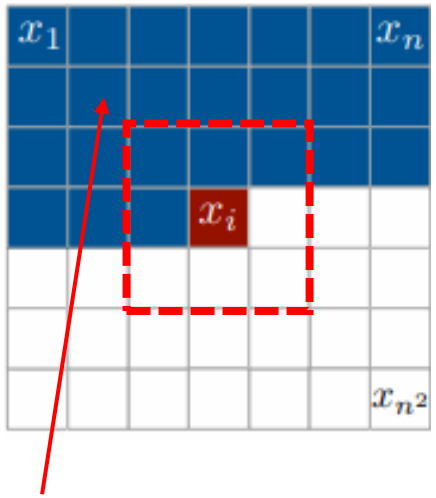
- It's very slow
- Row-by-row LSTMs might struggle to capture spatial context (pixels right above are "far away")
- Many practical improvements and better architectures are possible!



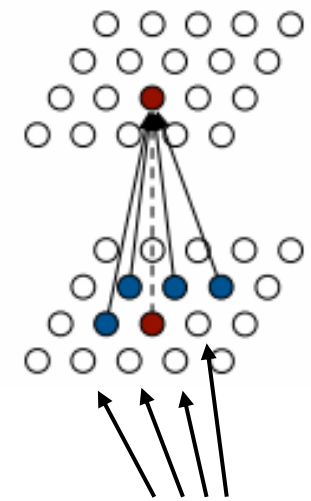
Van den Oord et al. **Pixel Recurrent Neural Networks**. 2016.

PixelCNN

Idea: make this much faster by not building a full RNN over all pixels, but just using a convolution to determine the value of a pixel based on its neighborhood



this pixel still influences x_i!
why?



these are **masked out** because they haven't been generated yet

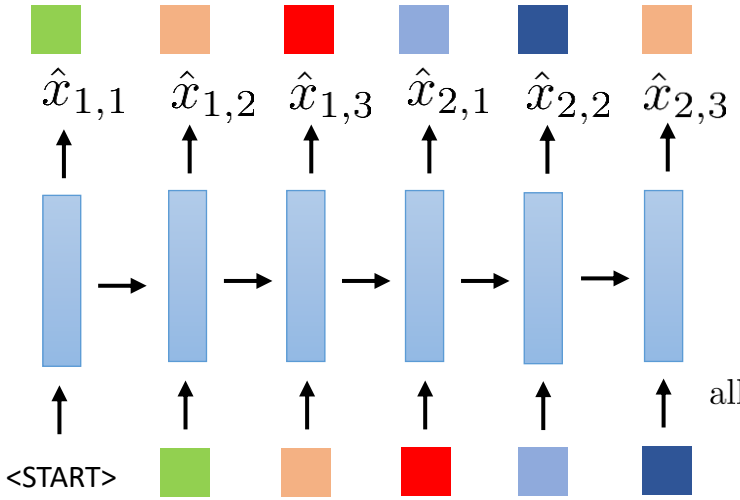
Question: can we parallelize this?

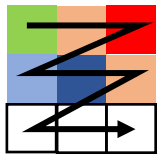
During **training**?

During **generation**?

Van den Oord et al. **Pixel Recurrent Neural Networks**. 2016.

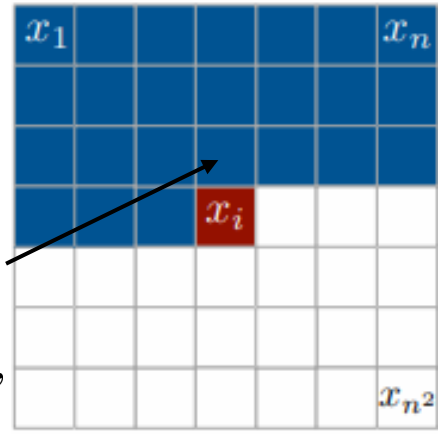
Pixel Transformer





this pixel very far from x_i for an RNN

all pixels are **equally "close"** for self-attention

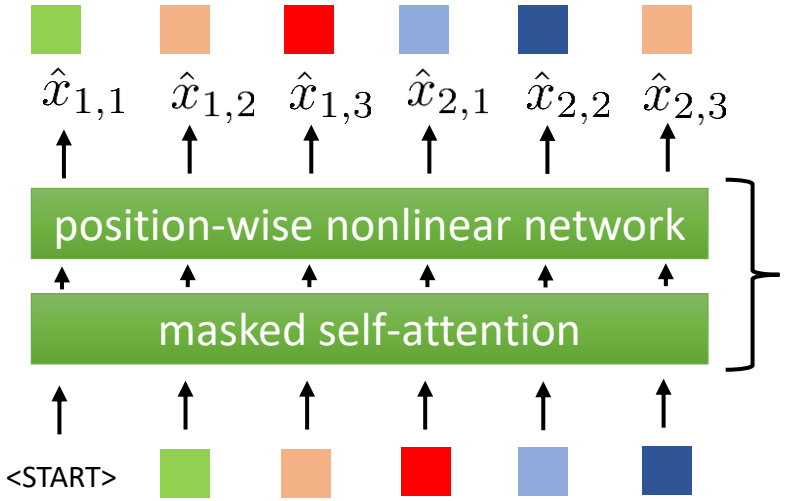


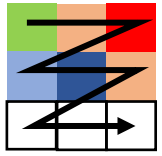
Problem: the number of pixels can be **huge**

attention can become prohibitively expensive

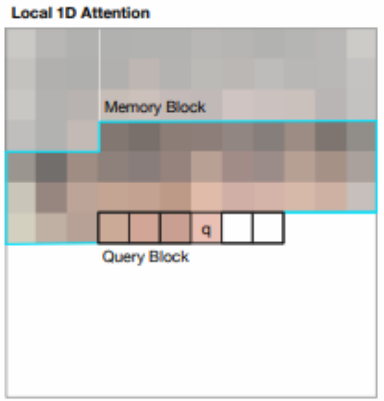
Idea: only compute attention for pixels that are not too far away

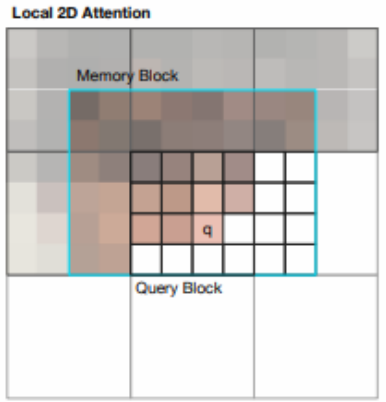
(looks a little like PixelCNN)





repeated **N**x





Parmar et al. **Image Transformer**. 2018.

PixelRNN vs. Pixel Transformer

PixelRNN

Transformer

All models trained on CIFAR-10

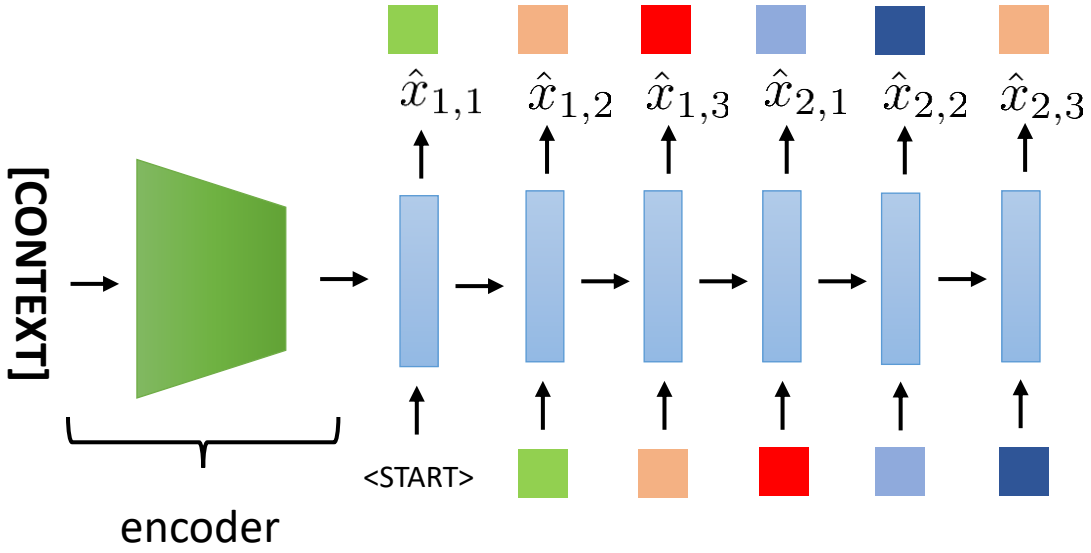
Parmar et al. **Image Transformer**. 2018.

Conditional autoregressive models

What if we want to generate something **conditioned** on another piece of information?

Examples:

- Generate images of specific types of objects (e.g., categories)
- Generate distributions over actions for imitation learning conditioned on the observation
- Many other examples!



Just like conditional language models!

Encoder can be **extremely simple** (e.g., generate images of a class)

Encoder can be **extremely complex** (e.g., multimodal policy in IL)

Conditional autoregressive models

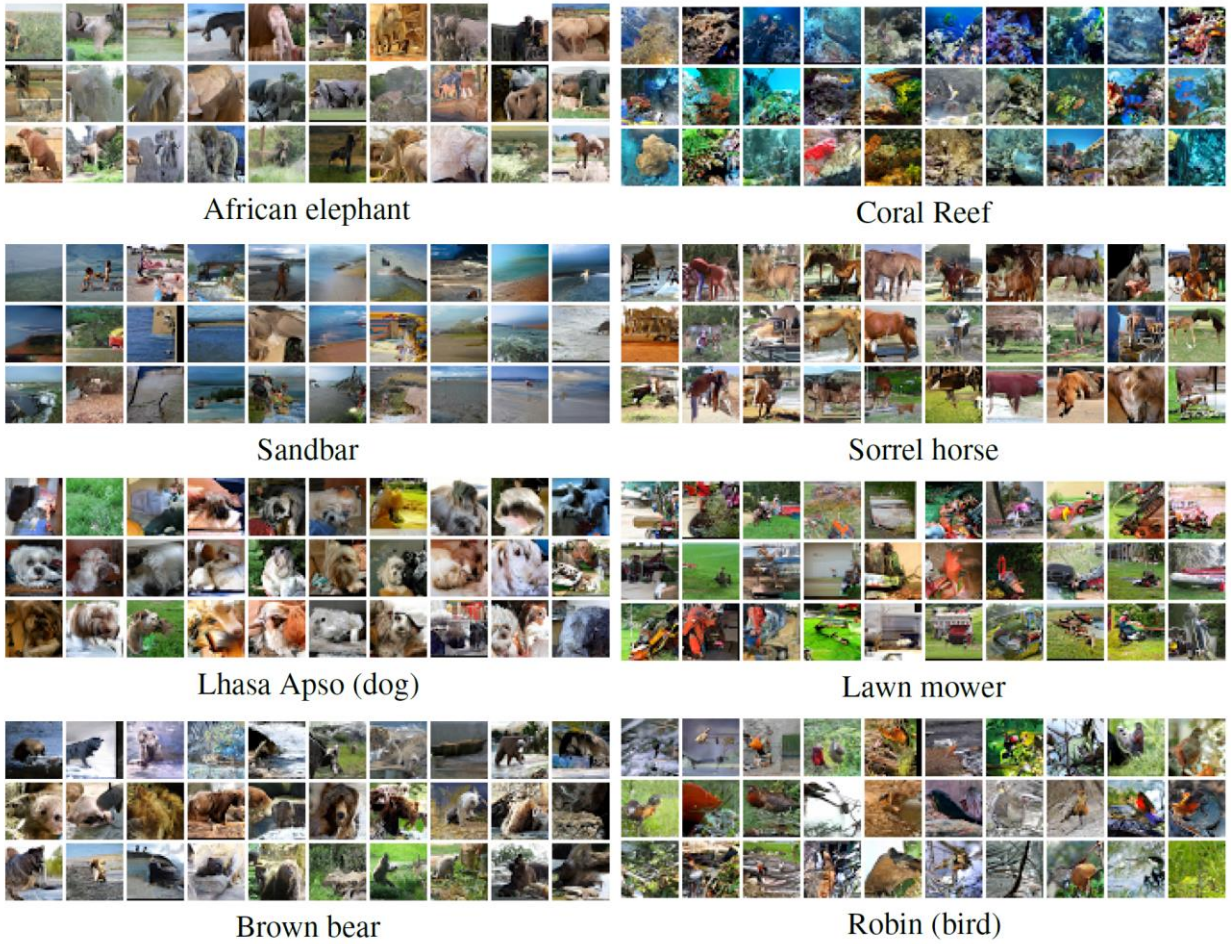


Figure 3: Class-Conditional samples from the Conditional PixelCNN.

Van den Oord et al. **Pixel Recurrent Neural Networks**. 2016.

Tradeoffs and considerations

- Autoregressive generative models are “language models” for other types of data
  - Though more accurate to say that language models are just a special type of autoregressive generative model

- Can represent autoregressive models in many different ways
  - RNNs (e.g., LSTMs)
  - Local context models like PixelCNNs
  - Transformers

- Tradeoffs compared to other models we’ll learn about:

  + provide full distribution with probabilities

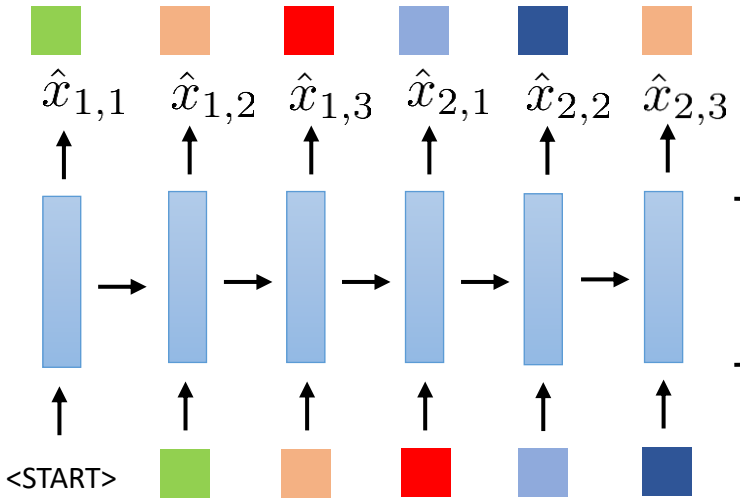
  + conceptually very simple

  - very slow for large datapoints (e.g., images)

  - generally limited in image resolution

Autoencoders

A 30,000 ft view…

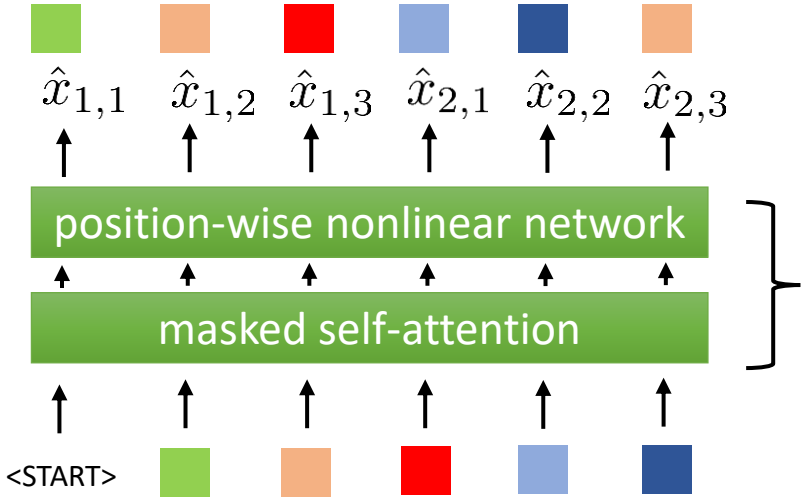


goal is to produce the **same** image

some structure here makes this task of "reconstructing" the input image nontrivial

In this case, it's the fact that each pixel must be constructed from **preceding** pixels

image goes in as input



structure comes from **masking** in the self-attention operator (otherwise this would be trivial!)

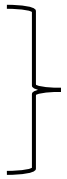
remember BERT…

A 30,000 ft view…

A general design for generative models?

loss

model



some structure here makes this task of “reconstructing” the input image nontrivial

i.e., prevents learning an “identity function”

Examples of structure that we’ve seen:

- RNN/LSTM sequence models that must predict a pixel’s value based only on “previous” pixels
- “PixelCNN” models that must predict a pixel’s value based on a (masked) neighborhood
- Pixel transformer, which must make predictions based on **masked** self-attention

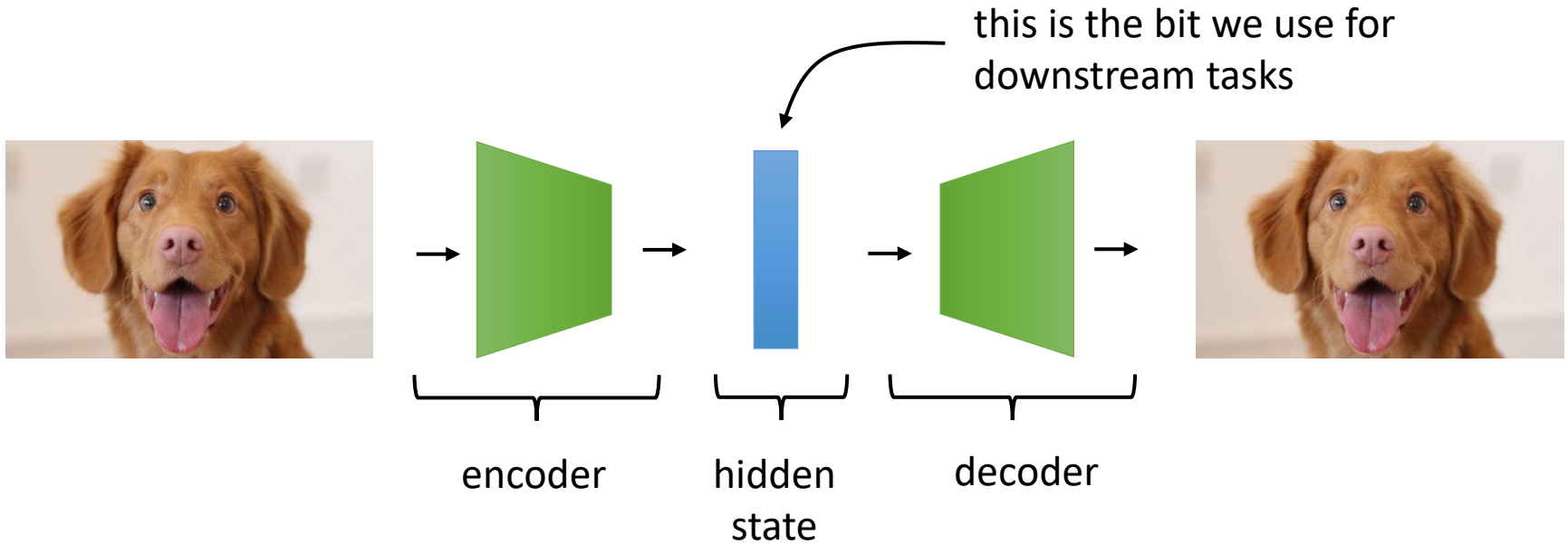
This is all **spatial** structure, can we use more abstract structure instead?

The autoencoder principle

Basic idea: train a network that **encodes** an image into some **hidden state**, and then **decodes** that image **as accurately as possible** from that **hidden state**

Such a network is called an **autoencoder**

Forcing structure: something about the design of the model, or in the data processing or regularization, must force the autoencoder to learn a **structured** representation



The types of autoencoders

Forcing structure: something about the design of the model, or in the data processing or regularization, must force the autoencoder to learn a **structured** representation

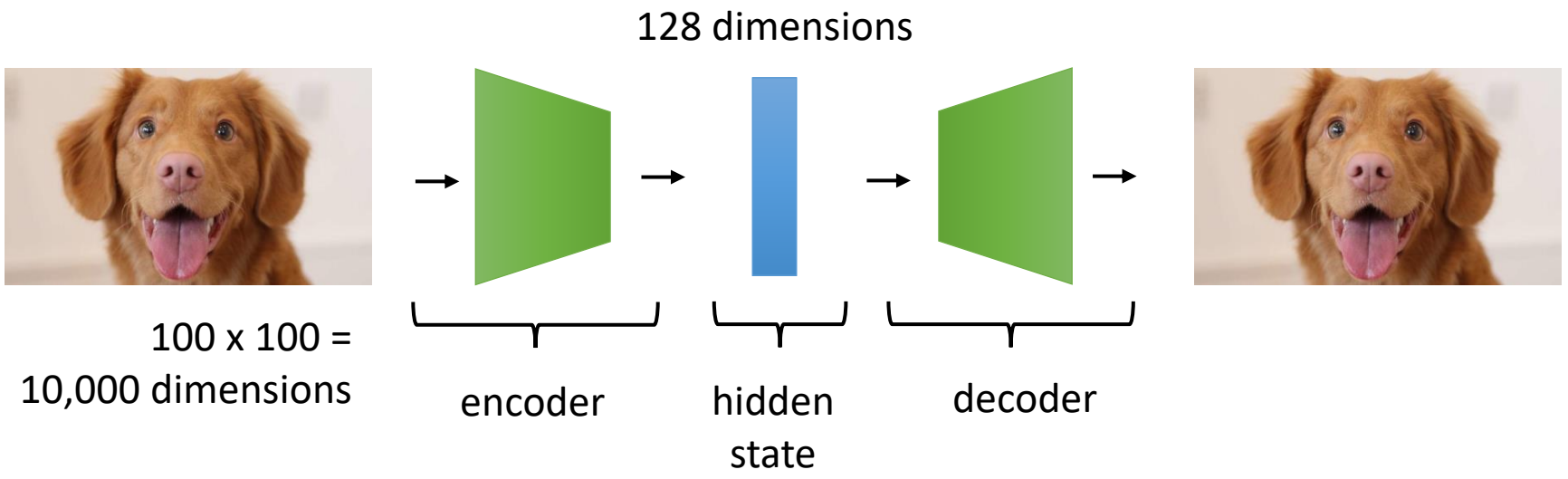
Dimensionality: make the **hidden state** smaller than the **input/output**, so that the network must **compress** it

Sparsity: force the **hidden state** to be sparse (most entries are zero), so that the network must **compress** the input

Denoising: corrupt the **input** with **noise**, forcing the autoencoder to learn to distinguish **noise from signal**

Probabilistic modeling: force the **hidden state** to agree with a **prior distribution** (this will be covered next time)

(Classic) Bottleneck autoencoder

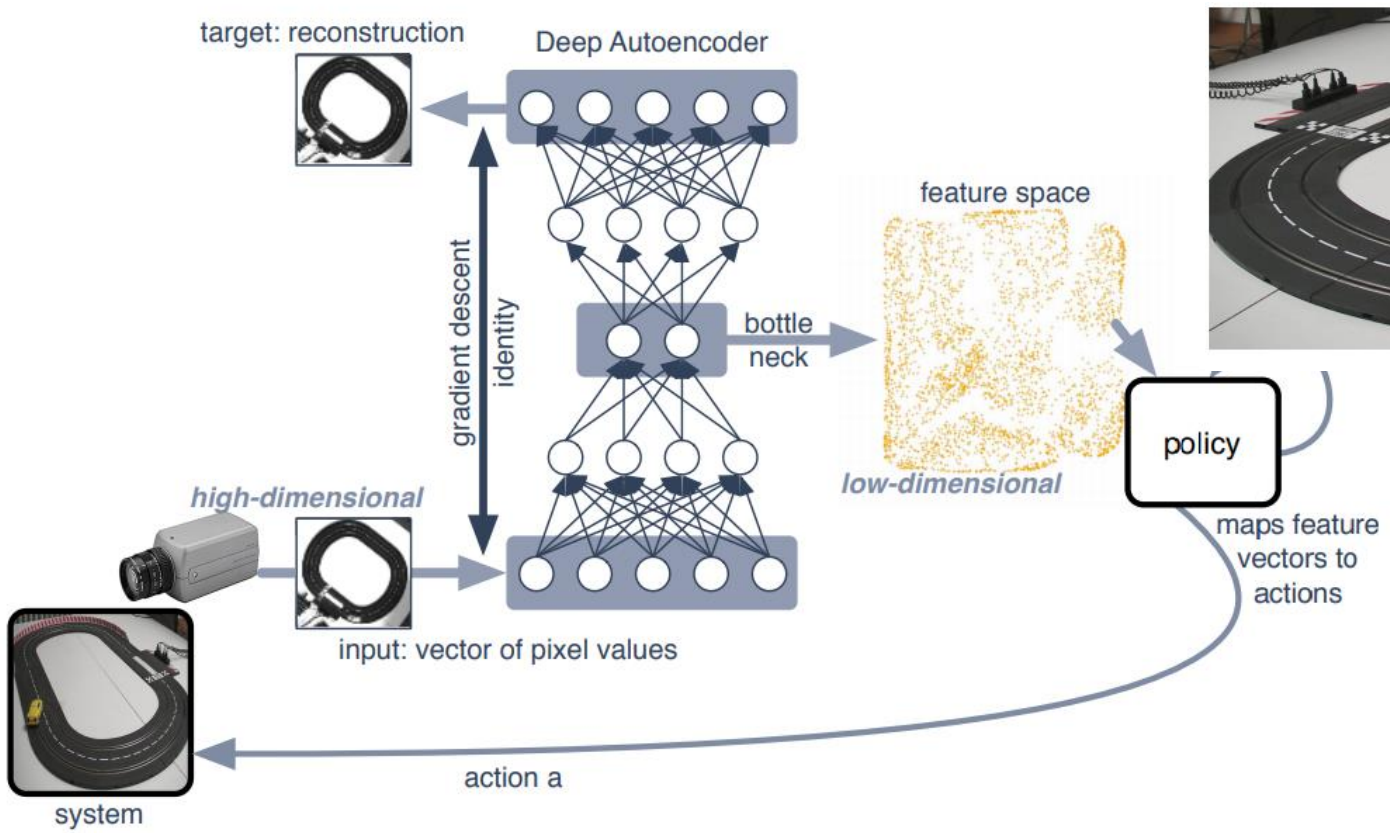


This has some interesting properties:

- If both encoder and decoder are **linear** (which is usually not very interesting), this exactly recovers PCA
- Can be viewed as "non-linear dimensionality reduction" – could be useful simply because dimensionality is lower and we can use various algorithms that are only tractable in low-dimensional spaces (e.g., discretization)

Today, this design is rather antiquated and rarely used, but good to know about historically

Bottleneck autoencoder example



Lange & Riedmiller. **Autonomous reinforcement learning from raw visual data**. 2012.

Sparse autoencoder

Idea: can we describe the input with a small set of "attributes"?

This might be a more **compressed** and **structured** representation

Aside:

This idea originated in neuroscience, where researchers believe that the brain uses **sparse** representations (see "sparse coding")

Pixel (0,0): #FE057D
Pixel (0,1): #FD0263
Pixel (0,2): #E1065F
⋮

NOT structured

"dense": most values non-zero

Idea: "sparse" representations are going to be more structured!

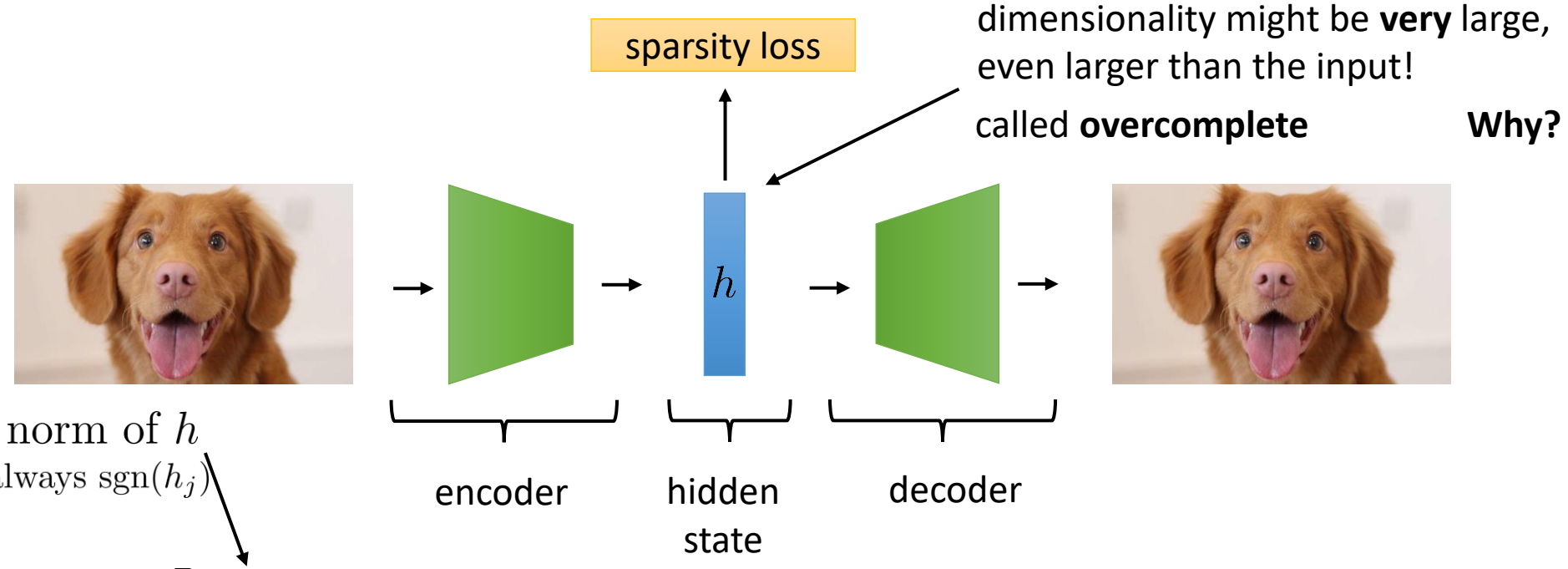
has_ears: 1
has_wings: 0
has_wheels: 0
⋮

very structured!

"sparse": most values are zero

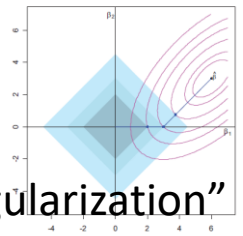
there are many possible "attributes," and most images don't have most of the attributes

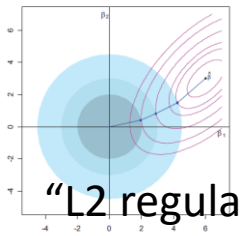
Sparse autoencoder



ℓ_1 norm of h
gradient is always $\text{sgn}(h_j)$

simple sparsity loss: $\sum_{j=1}^{D} |h_j|$


"L1 regularization"

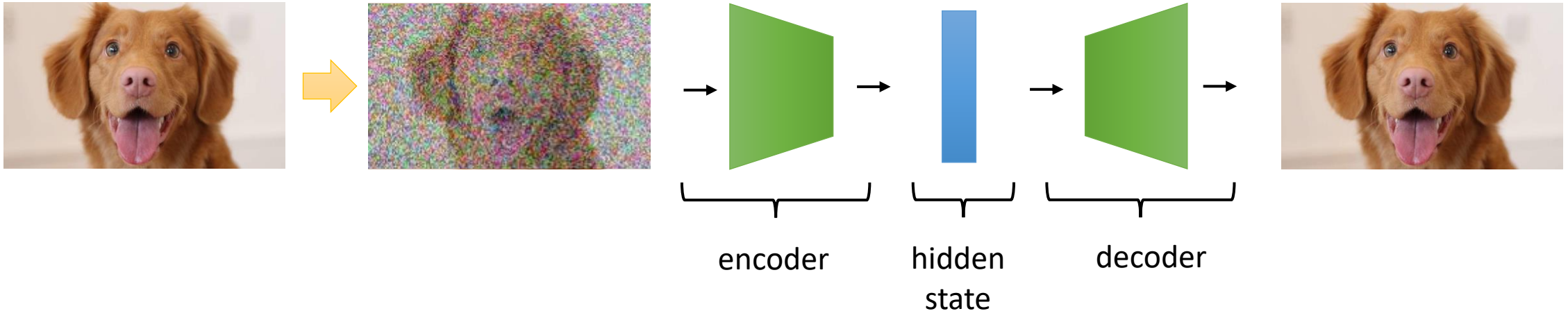

"L2 regularization"

There are other kinds of sparsity losses/models:

- Lifetime sparsity
- Spike and slab models

Denoising autoencoder

Idea: a good model that has learned meaningful structure should “fill in the blanks”



There are **many variants** on this basic idea, and this is one of the most widely used simple autoencoder designs

The types of autoencoders

Forcing structure: something about the design of the model, or in the data processing or regularization, must force the autoencoder to learn a **structured** representation

Dimensionality: make the **hidden state** smaller than the **input/output**, so that the network must **compress** it

+ very simple to implement

- simply reducing dimensionality often does not provide the structure we want

Sparsity: force the **hidden state** to be sparse (most entries are zero), so that the network must **compress** the input

+ principled approach that can provide a "disentangled" representation

- harder in practice, requires choosing the regularizer and adjusting hyperparameters

Denoising: corrupt the **input** with **noise**, forcing the autoencoder to learn to distinguish **noise from signal**

+ very simple to implement

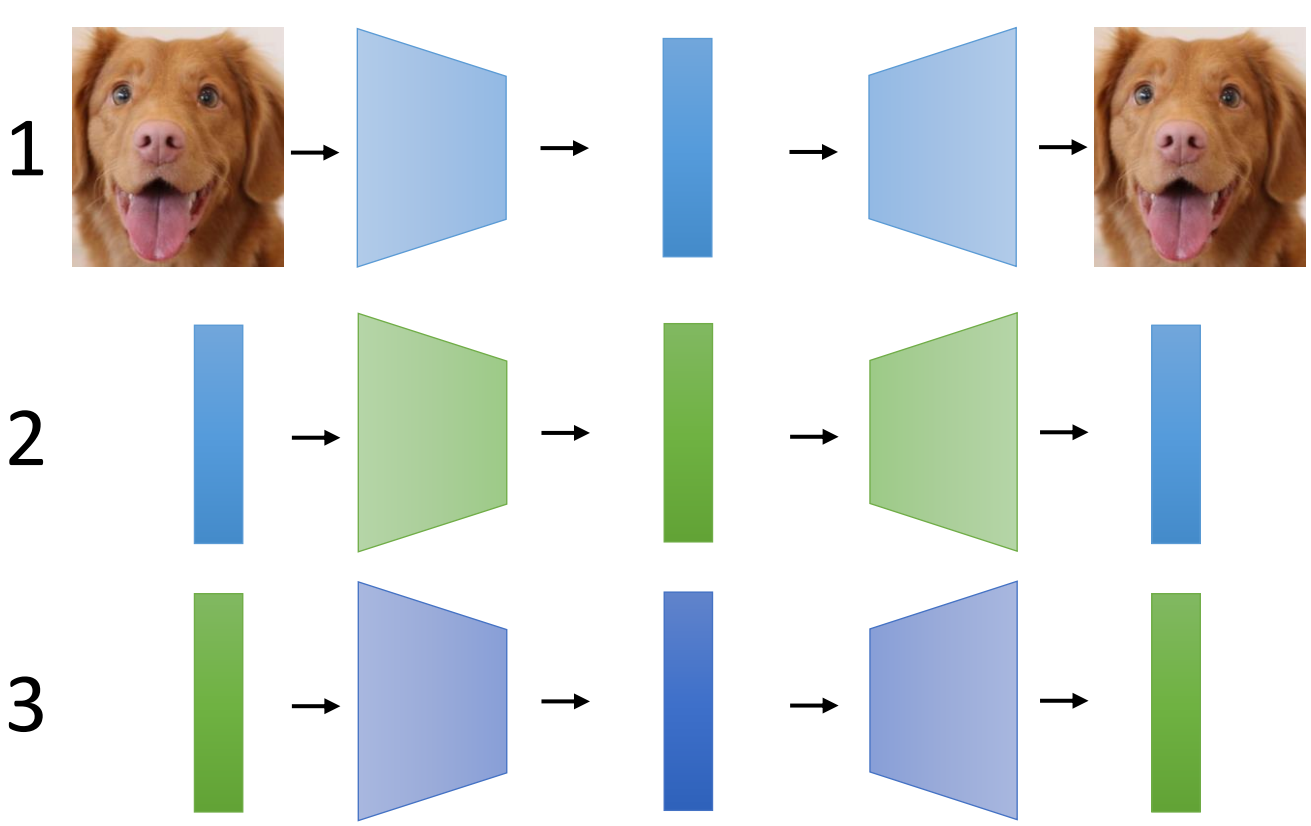
- not clear which layer to choose for the bottleneck, many ad-hoc choices (e.g., how much noise to add)

Probabilistic modeling: force the **hidden state** to agree with a **prior distribution** (this will be covered next time)

We'll discuss this design in much more detail in the next lecture!

Layerwise pretraining

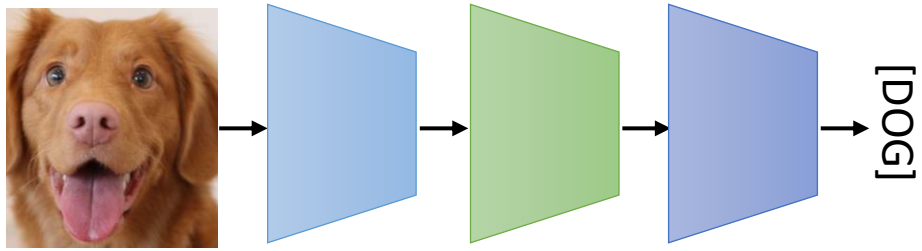
The early days of deep learning…



For a while (2006-2009 or so), this was one of the dominant ways to train **deep** networks

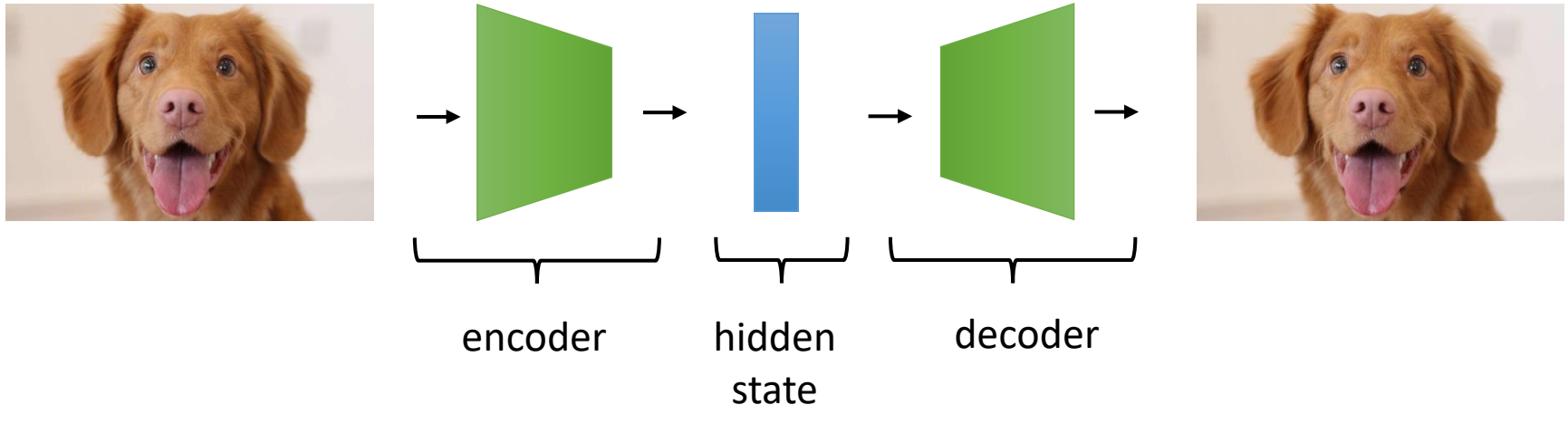
Then we got a lot better at training deep networks end-to-end (ReLU, batch norm, better hyperparameter tuning), and largely stopped doing this

Correspondingly, autoencoders became less important, but they are still useful!



Autoencoders today

- Much **less** widely used these days because there are better alternatives
  - **Representation learning:** VAEs, contrastive learning
  - **Generation:** GANs, VAEs, autoregressive models
- Still a viable option for "quick and dirty" representation learning that is very fast and can work OK
- **Big problem:** sampling (generation) from an autoencoder is hard, which limits its uses
  - The variational autoencoder (VAE) addresses this, and is the most widely used autoencoder today – we will cover this next time!

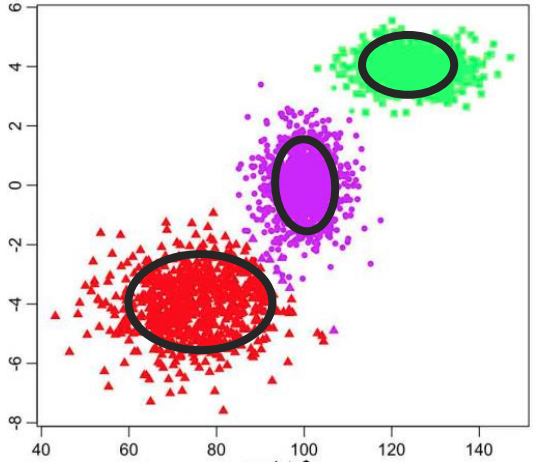


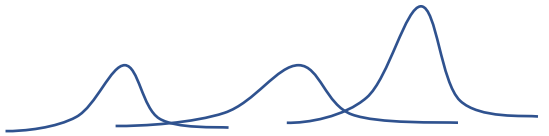
Latent Variable Models

Latent variable models

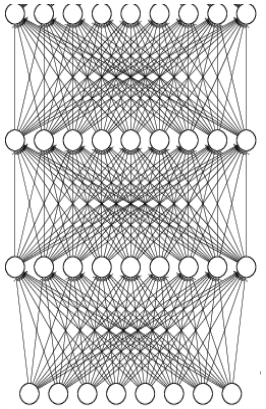
$$p(x) = \sum_z p(x|z)p(z)$$

mixture element

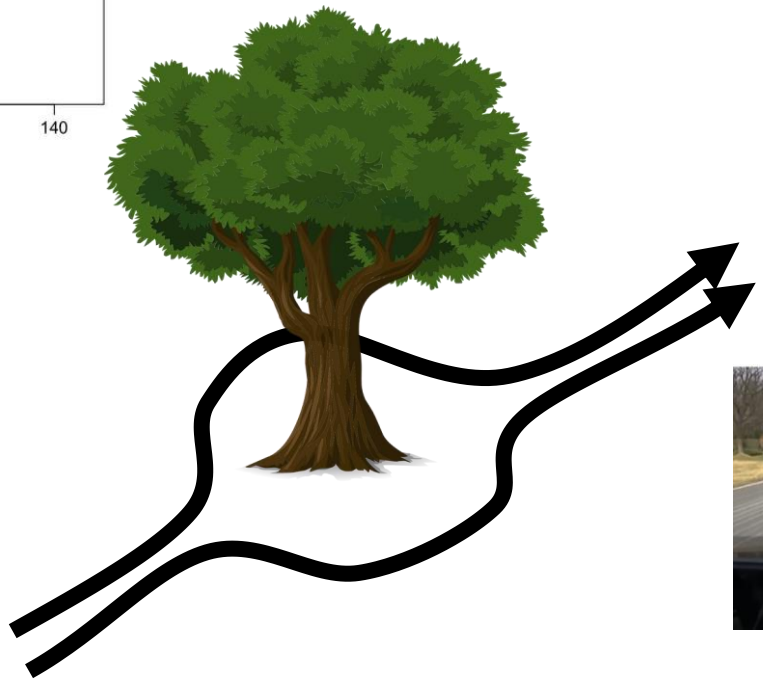


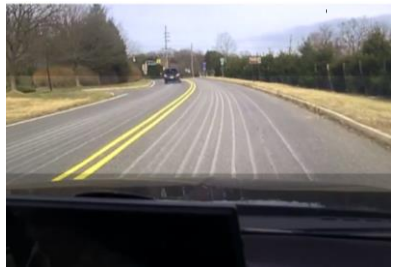


$$w_1, \mu_1, \Sigma_1, \ldots, w_N, \mu_N, \sigma_N$$



$$p(y|x) = \sum_z p(y|x,z)p(z)$$



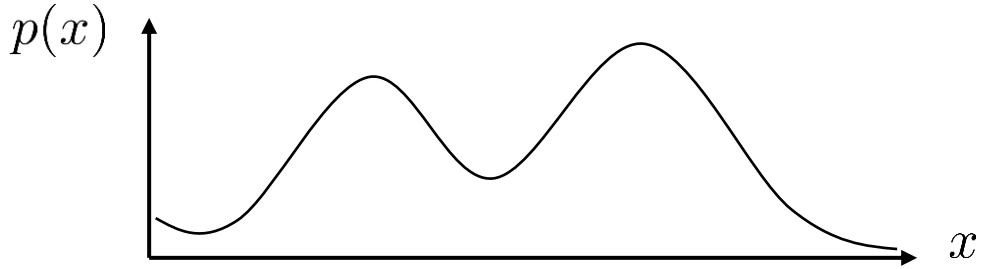


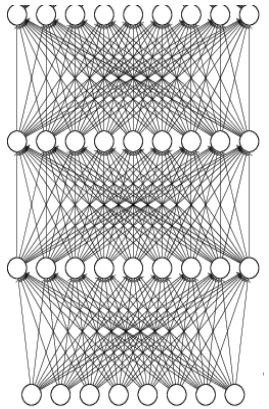
Latent variable models in general

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

"easy" distribution
(e.g., conditional Gaussian)

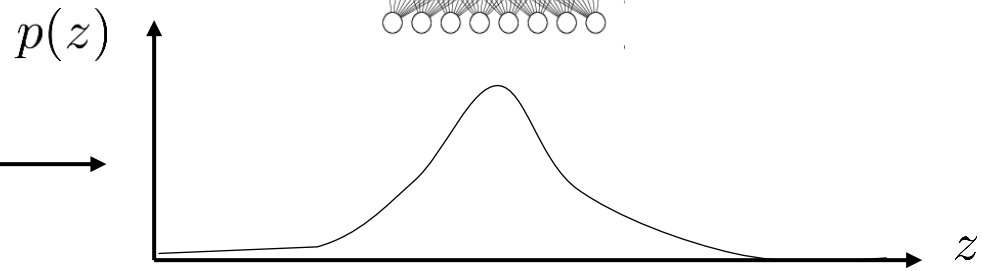
"easy" distribution
(e.g., Gaussian)





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

"easy" distribution
(e.g., Gaussian)



How do we train latent variable models?

the model: $p_\theta(x)$

the data: $\mathcal{D} = \{x_1, x_2, x_3, \ldots, x_N\}$

maximum likelihood fit:

$$\theta \leftarrow \arg\max_\theta \frac{1}{N} \sum_i \log p_\theta(x_i) \qquad p(x) = \int p(x|z)p(z)dz$$

$$\theta \leftarrow \arg\max_\theta \frac{1}{N} \sum_i \log \left(\int p_\theta(x_i|z)p(z)dz \right)$$

completely intractable

Estimating the log-likelihood

alternative: *expected* log-likelihood:

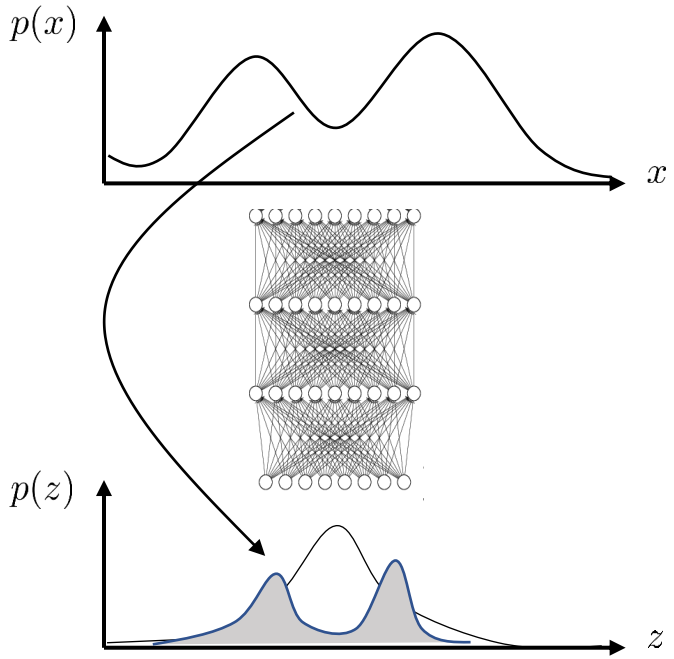
$$\theta \leftarrow \arg\max_{\theta} \frac{1}{N} \sum_{i} E_{z \sim p(z|x_i)} [\log p_\theta(x_i, z)]$$

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

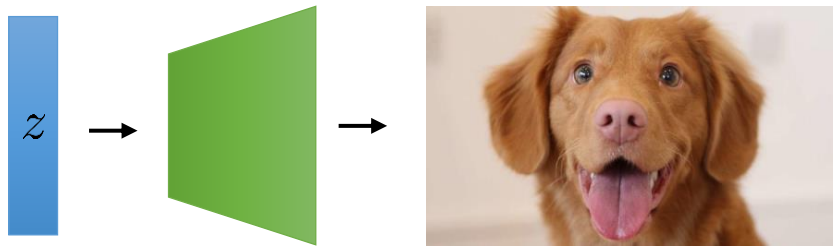
this is called **probabilistic inference**

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 $p(z|x_i)$



Latent variable models in deep learning



$p(z)$ $p_\theta(x|z)$

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

A latent variable deep generative model is (usually) just a model that turns random numbers into valid samples (e.g., images)

Please don't tell anyone I said this, it destroys the mystique

There are many types of such models: VAEs, GANs, normalizing flows, etc.

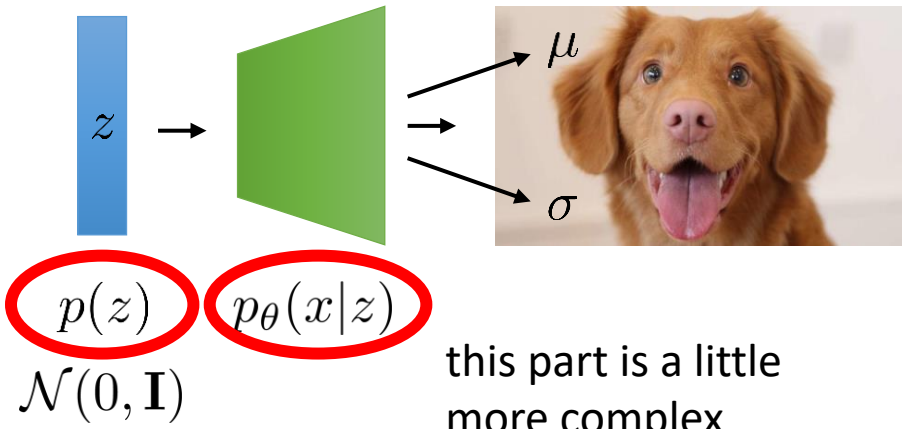
Using the model for **generation**:

1. sample $z \sim p(z)$ "generate a vector of random numbers"
2. sample $x \sim p(x|z)$ "turn that vector of random numbers into an image"

Today: how do we represent and use this

Next time: how do we train this

Representing latent variable models



this part is easy, just generate (e.g.) Gaussian random numbers

this part is a little more complex

How do we represent the distribution over x?

Option 1: Pixels are continuous-valued

$$p_\theta(x|z) = \mathcal{N}(\mu_\theta(z); \sigma_\theta(z))$$

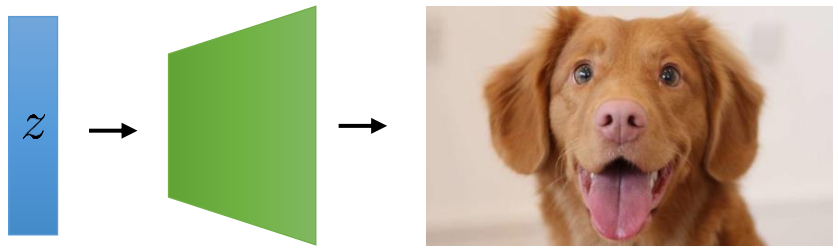
mean is a neural net function

variance is (optionally) a neural net function

easy choice: let σ just be a constant either a learned constant (independent of z) or chosen manually (e.g., 1)

This just reduces to MSE loss!

Representing latent variable models



$p(z)$ $p_\theta(x|z)$

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

How do we represent the distribution over x?

Option 2: Pixels are discrete-valued

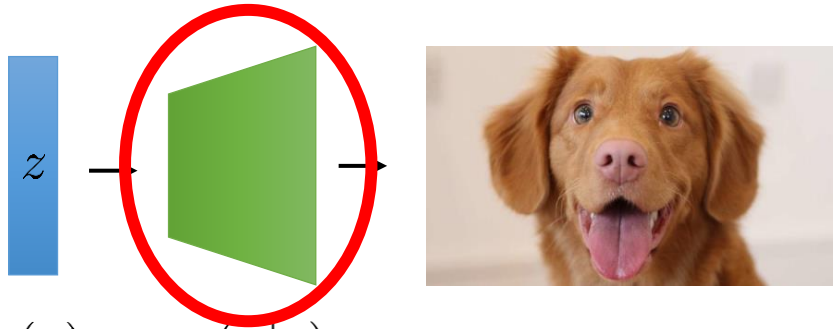
Could just a 256-way softmax, just like in PixelRNN or PixelCNN!

(this works very well, but is a little bit slow)

Other choices (not covered in this lecture): discretized logistic, binary cross-entropy

especially common for best performing models

Representing latent variable models



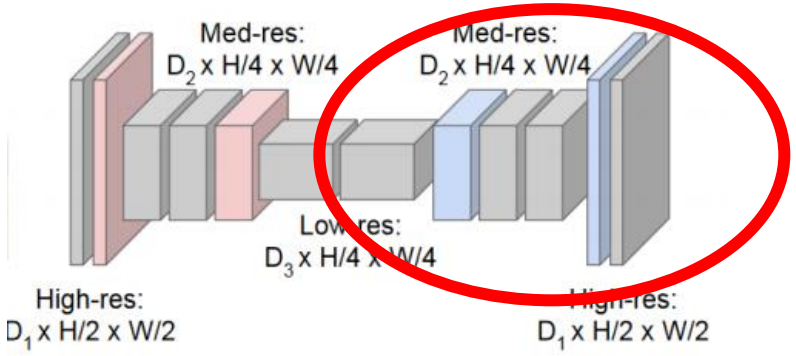
$p(z)$ $p_\theta(x|z)$ what architecture should we use?

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

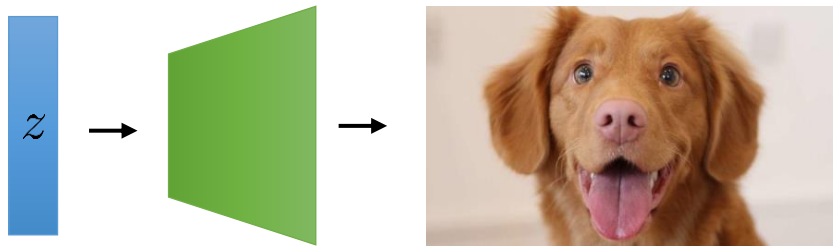
Easy choice: just a big fully connected network (linear layers + ReLU)

works well for tiny images (e.g., MNIST) or non-image data

Better choice: transpose convolutions



Training latent variable models



$p(z)$ $p_\theta(x|z)$

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

1a. sample $z \sim p(z|x_i)$

1b. reduce $-\log p(x_i|z)$ with SGD

variational autoencoders (VAEs)

Three basic choices:

1. Perform inference to figure out $p(z|x_i)$ for each training image x_i

   Then minimize *expected* NLL $E_{p(z|x_i)}[-\log p(x_i|z)]$

2. Use an *invertible* mapping z to x **normalizing flows**

3. Match the distribution $E_{z\sim p(z)}[p_\theta(x|z)]$ to data distribution

generative adversarial networks (GANs)