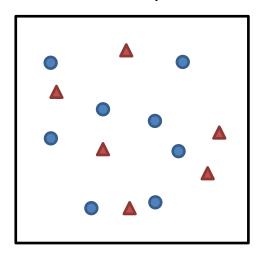
# Neural Networks and Deep Learning

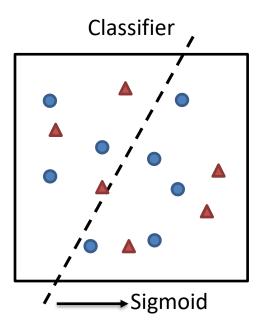
Autoencoders

#### **MOTIVATION**

## Drawing lines in space

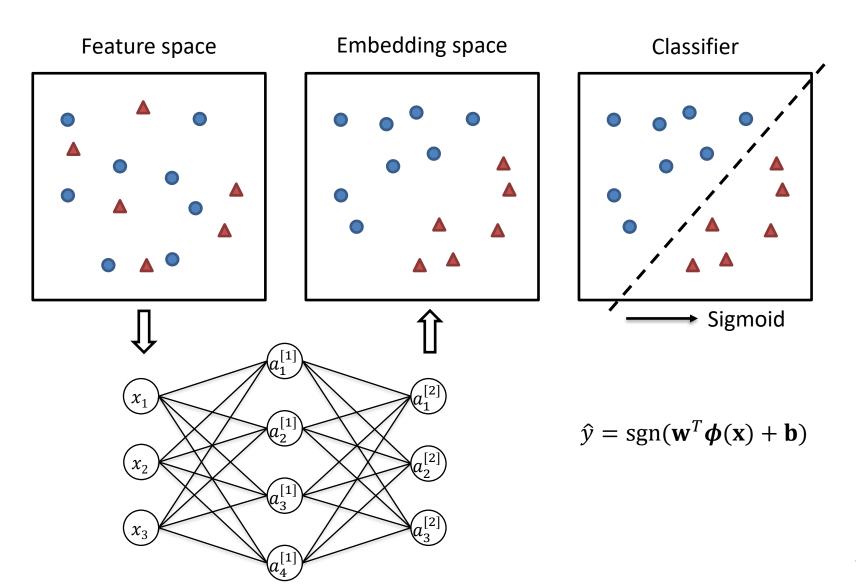
#### Feature space



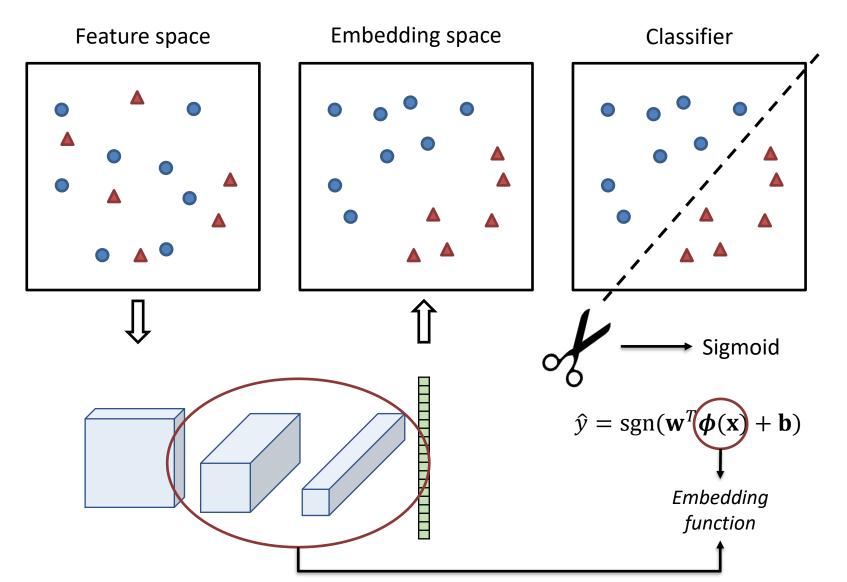


$$\hat{y} = \operatorname{sgn}(\mathbf{w}^T \mathbf{x} + \mathbf{b})$$

## Drawing lines in space

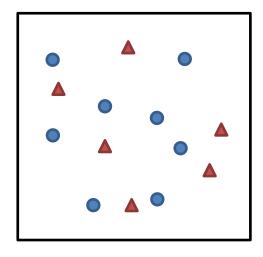


## Drawing lines in space

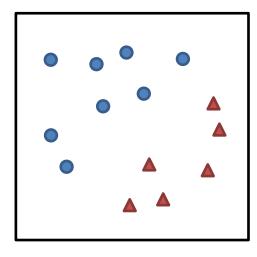


## **Embedding**

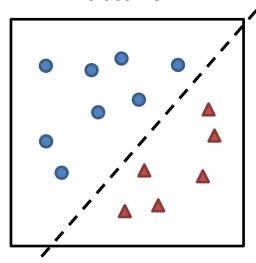
Feature space



Embedding space



Classifier



An **embedding** is a new (intermediate) representation of our original features (data).

The final **embedding space** is typically a lower-dimensional space than our original features.

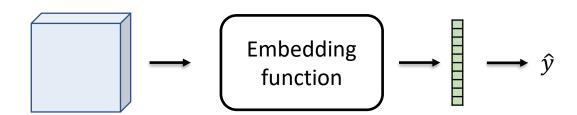
The embedding process converts our data in a way that it is easier to solve the problem at hand.

## **Embedding**

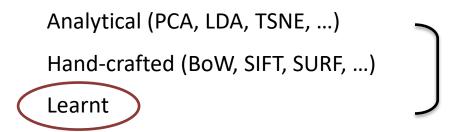
Embedding
Feature extraction
Projecting data into a new space
Representation learning
Feature design / learning

Are all equivalent expressions (in our scenario)

•••



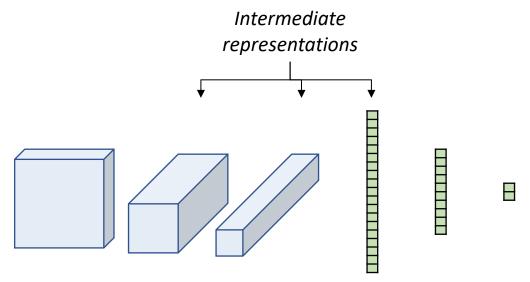
Feature design / learning can be driven by data and/or previous knowledge



and reused across models

## **Embedding**

In deep neural networks, we repeatedly embed (project) our data into new spaces

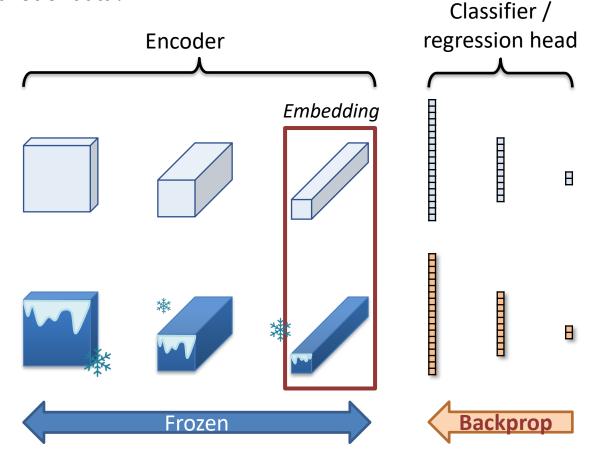


The right embedding to use, depends on the problem we are solving.

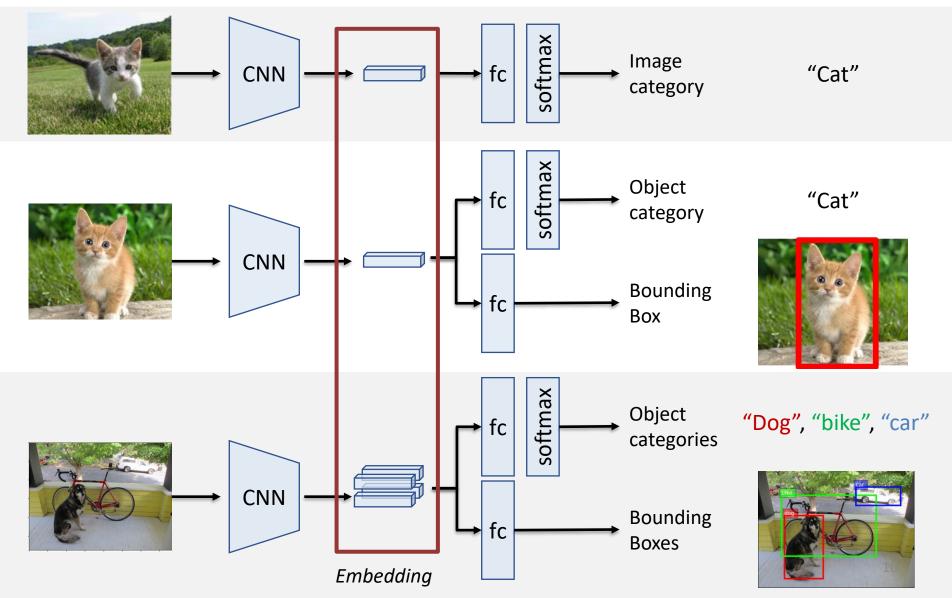
In Deep Learning, this process is end-to-end (task driven), and data driven

## Reusing embeddings

Learning features is data hungry... How can we get an embedding when we lack a lot of data?



## Same pattern...



## Supervised Learning









## Semi-Supervised Learning







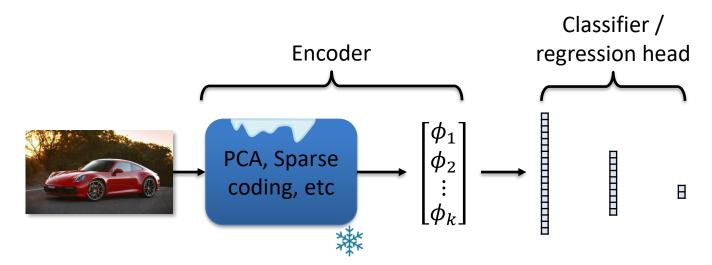




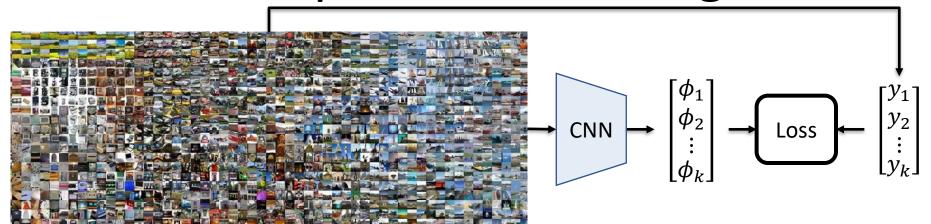
## Unsupervised learning



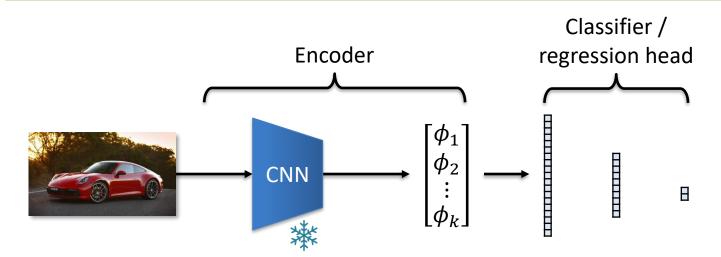
Learning the underlying structure of the data over non-labelled samples, would make it easier to learn a supervised model afterwards



## Unsupervised learning



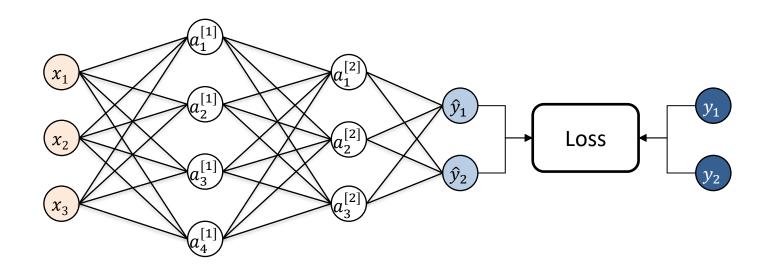
A different idea, is to somehow create a supervisory signal from data that do not have annotations...



How can we create useful embeddings without annotated data?

#### **AUTOENCODERS**

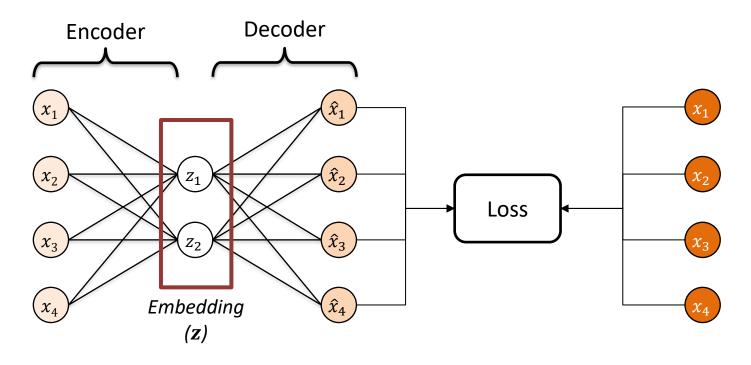
## Training a neural network



Given a training set:  $(\mathbf{x}^{(1)}, \mathbf{y}^{(1)})$ ,  $(\mathbf{x}^{(2)}, \mathbf{y}^{(2)})$ ,  $(\mathbf{x}^{(3)}, \mathbf{y}^{(3)})$ , ...

Adjust parameters **W** (of every layer) to make:  $\hat{\mathbf{y}}^{(i)} = f_{\mathbf{W}}(\mathbf{x}^{(i)}) \approx \mathbf{y}^{(i)}$ 

#### Autoencoder

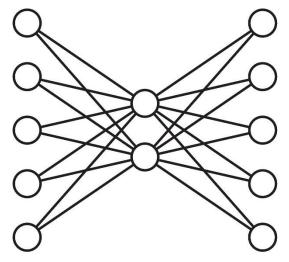


Given a training set without annotations:  $\mathbf{x}^{(1)}$ ,  $\mathbf{x}^{(2)}$ ,  $\mathbf{x}^{(3)}$ , ...

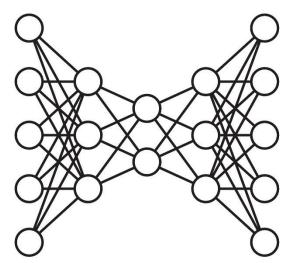
Adjust parameters  $\mathbf{W}$  (of every layer) to make:  $f_{\mathbf{W}}(\mathbf{x}^{(i)}) \approx \mathbf{x}^{(i)}$ 

How can we learn a useful representation (z)?

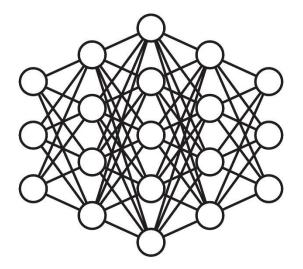
## Types of autoencoders



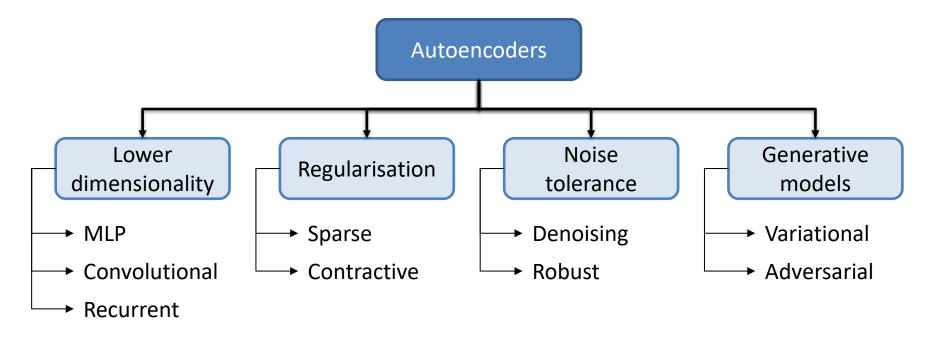
(a) Shallow undercomplete



(b) Shallow overcomplete



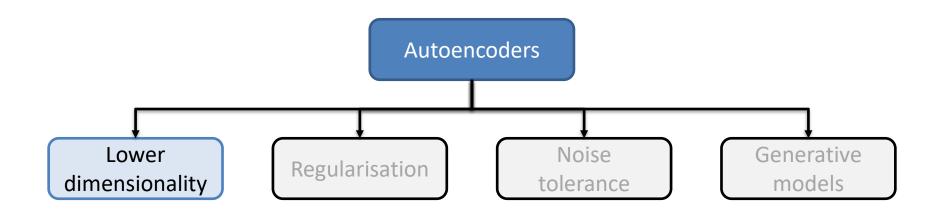
### Autoencoders taxonomy



The network is trained to output (reconstruct) the input.

This has a trivial solution (learn the identify function) unless we

- constrain the number of units in embedding layer (compressed representation)
- constrain the embedding layer to be sparse
- introduce a small change in the input and learn to undo it
- force some particular distribution for the embeddings



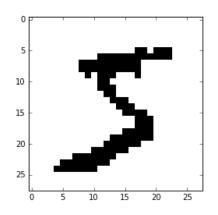
Compression – learning embeddings of lower dimensionality

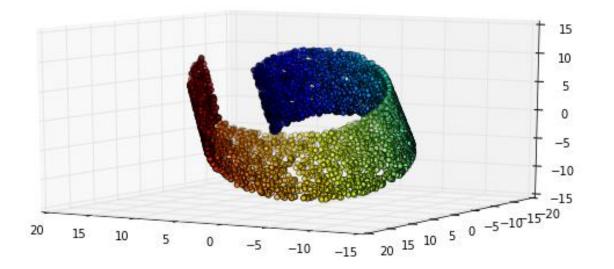
#### **COMPRESSION**

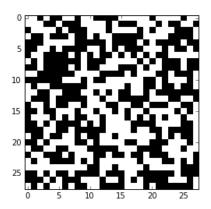
#### Motivation

Think about the handwritten digits (MNIST) data

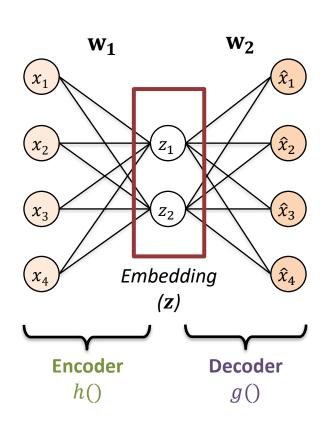
- 28 x 28 bitmaps
- Each pixel can either be black or white: {0, 1}<sup>784</sup> possible events
- We will never see most of the events
- The actual digits are a tiny fraction of the possible events
- It should be possible to describe our data with less features







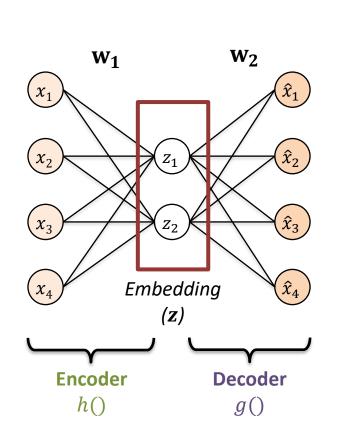
## Autoencoders: compression



$$J(\mathbf{w}) = \frac{1}{m} \sum_{i=1}^{m} L^{(i)}(\mathbf{w}) = \frac{1}{m} \sum_{i=1}^{m} L(f_{\mathbf{w}}(\mathbf{x}^{(i)}), \mathbf{y}^{(i)})$$

$$J(\mathbf{w}) = \frac{1}{m} \sum_{i=1}^{m} L^{(i)}(\mathbf{w}) = \frac{1}{m} \sum_{i=1}^{m} L\left(g_{\mathbf{w}_2}\left(\mathbf{h}_{\mathbf{w_1}}(\mathbf{x}^{(i)})\right), \mathbf{x}^{(i)}\right)$$

## Autoencoders: compression



$$J(\mathbf{w}) = \frac{1}{m} \sum_{i=1}^{m} L^{(i)}(\mathbf{w}) = \frac{1}{m} \sum_{i=1}^{m} L\left(g_{\mathbf{w}_2}\left(h_{\mathbf{w_1}}(\mathbf{x}^{(i)})\right), \mathbf{x}^{(i)}\right)$$

$$L\left(g_{\mathbf{w_2}}\left(\mathbf{h_{w_1}}(\mathbf{x}^{(i)})\right), \mathbf{x}^{(i)}\right) = L_{MSE} \|\mathbf{x}^{(i)} - \hat{\mathbf{x}}^{(i)}\|$$

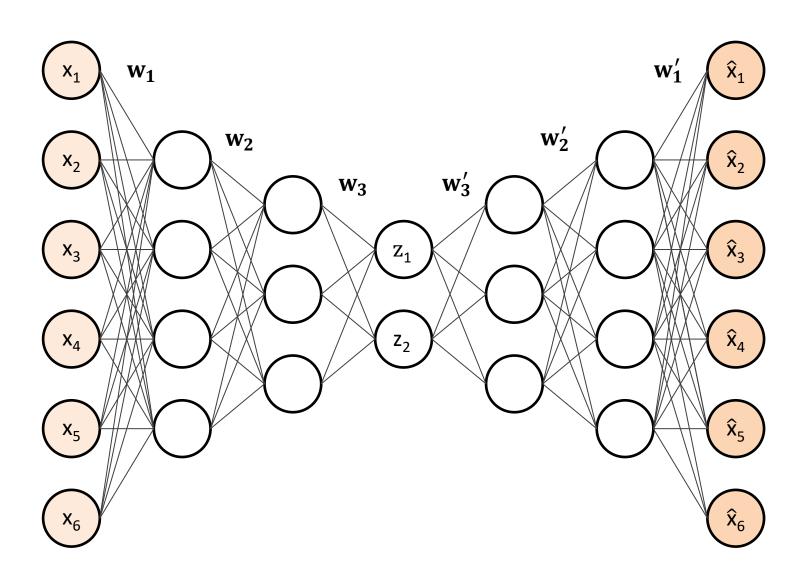
Or with L2 regularization:

$$L\left(g_{\mathbf{w}_{2}}\left(h_{\mathbf{w}_{1}}(\mathbf{x}^{(i)})\right),\mathbf{x}^{(i)}\right) = L_{MSE} \|\mathbf{x}^{(i)} - \hat{\mathbf{x}}^{(i)}\| + \lambda \sum_{k} \omega_{k}^{2}$$
$$\mathbf{w}_{1},\mathbf{w}_{2} = \{\omega_{k}\}$$

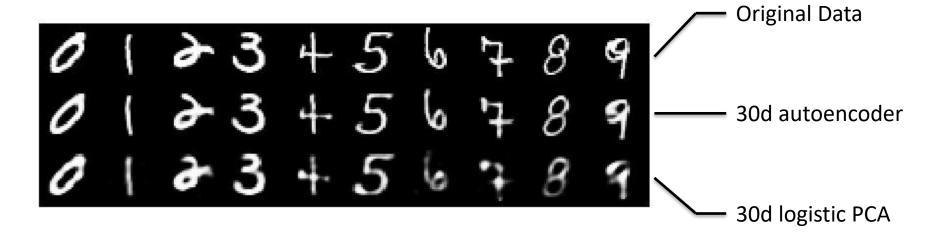
If encoder and decoder are symmetric, we can tie weights (use the same weights) on both sides to decrease number of parameters

$$\mathbf{w_1} = \mathbf{w_2}^T$$

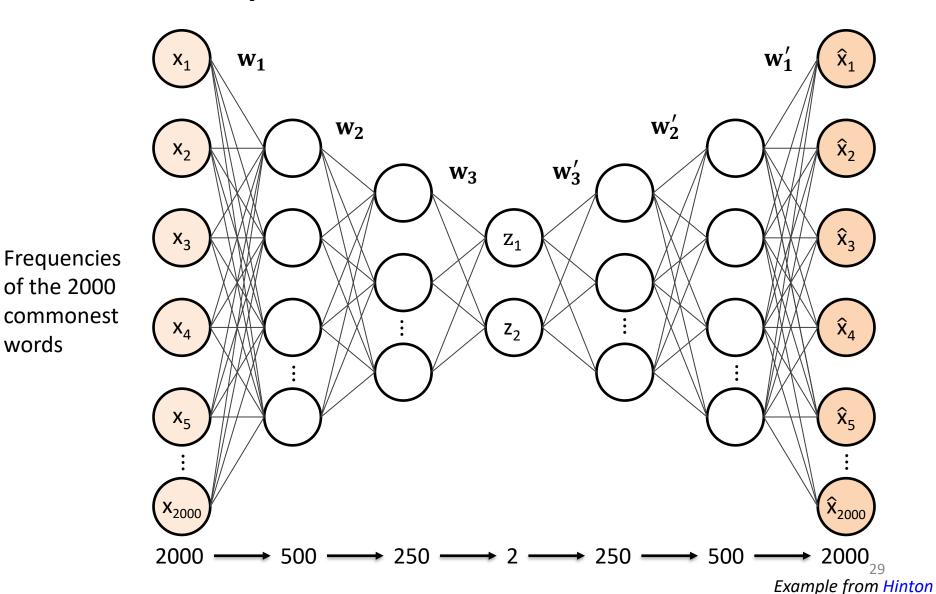
## Going deeper



## Comparison with PCA

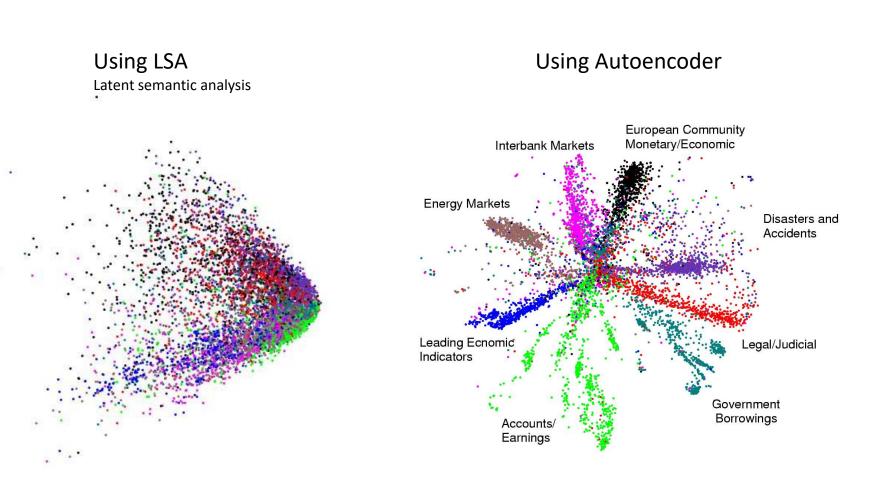


## Example: Document retrieval



words

## Example: Final 2D embeddings

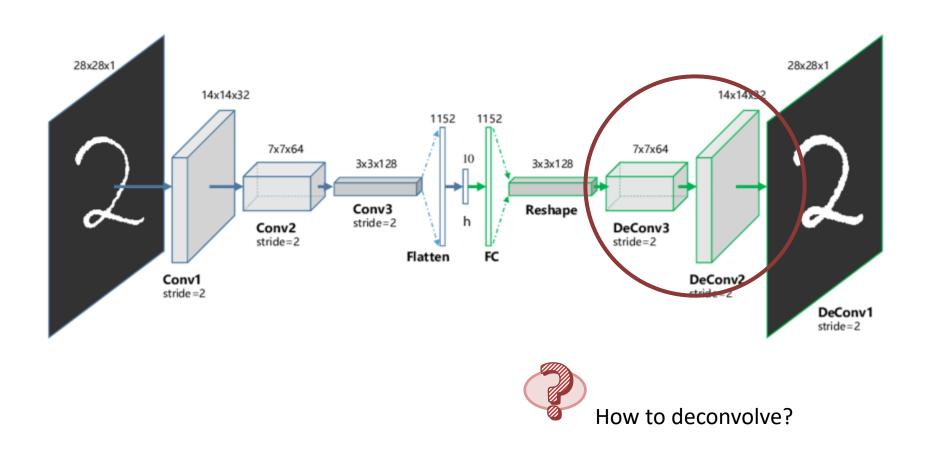


Different colours indicate different document clases – not used during training

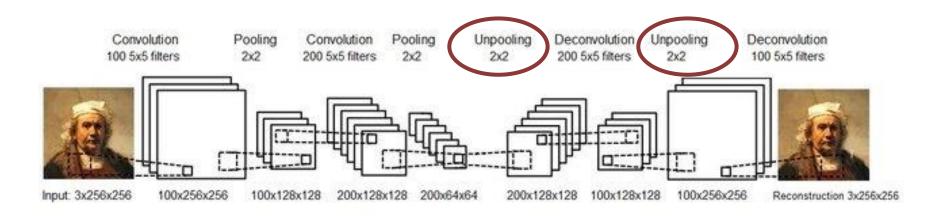
### O PyTorch Basic Autoencoder

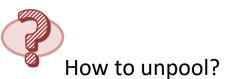
```
class autoencoder (nn. Module):
    def init (self):
        super(autoencoder, self). init ()
        self.encoder = nn.Sequential(
            nn.Linear(28 * 28, 128), nn.ReLU(True),
            nn.Linear(128, 64), nn.ReLU(True),
            nn.Linear(64, 12), nn.ReLU(True),
            nn.Linear(12, 3))
        self.decoder = nn.Sequential(
            nn.Linear(3, 12), nn.ReLU(True),
            nn.Linear(12, 64), nn.ReLU(True),
            nn.Linear(64, 128), nn.ReLU(True),
            nn.Linear(128, 28 * 28),
            nn.Tanh())
    def forward(self, x):
        x = self.encoder(x)
        x = self.decoder(x)
        return x
model = autoencoder().cuda()
criterion = nn.MSELoss()
```

#### Convolutional Autoencoders

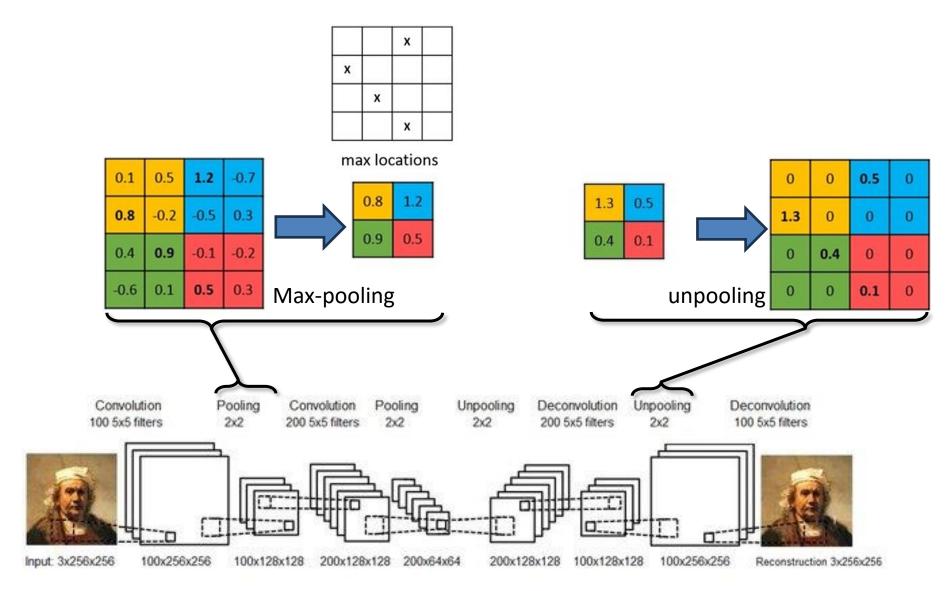


#### Convolutional Autoencoders





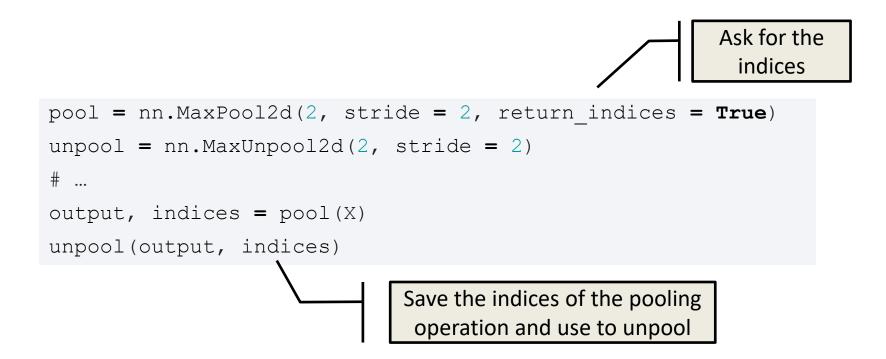
## Unpooling



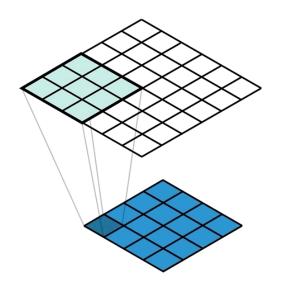


## Unpooling

MaxUnpool2d() - see the documentation



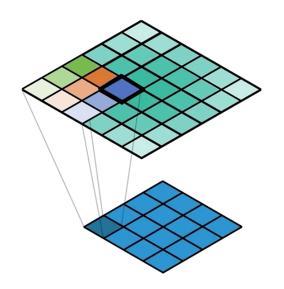
A transposed convolution (also called fractionally strided convolution or deconvolution) is the reverse process of convolution.



$w_1$	$w_2$	$w_3$
$W_4$	$w_5$	$W_6$
$w_7$	$w_8$	W <sub>9</sub>

The easiest way of thinking about it is to take each value in your input and distribute it (using the corresponding weights of a kernel) to a local region in the output

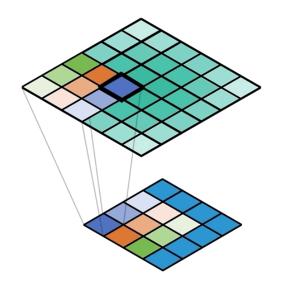
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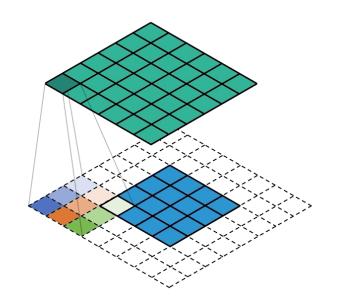
A transposed convolution (also called fractionally strided convolution or deconvolution) is the reverse process of convolution.



$w_1$	$W_2$	$W_3$
$w_4$	$w_5$	$W_6$
$w_7$	$w_8$	W <sub>9</sub>

Note how "distributing" the input values ends up being equivalent to applying a normal convolution with the transposed kernel

A transposed convolution (also called fractionally strided convolution or deconvolution) is the reverse process of convolution.

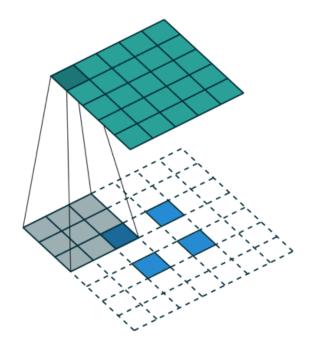


$w_1$	$w_2$	$W_3$
$w_4$	$w_5$	$W_6$
$w_7$	$w_8$	W <sub>9</sub>

Applying a forward convolution with a transposed kernel, actually results in a much smaller output. What we are really doing here is equivalent to this transposed convolution but with full padding

## Fractionally strided convolutions

The transpose of a convolution with stride s>1 involves an equivalent convolution with s<1. This is why transposed convolutions are sometimes called *fractionally strided convolutions*.



In the case of transposed convolutions invert the input and output sizes in the formula we defined earlier, and you get: o = (n-1)s - 2p + f

# Transponsed Convolutions (Deconvolutions)

Convolution:

$$n_{W/H}^{[l]} = \frac{n_{W/H}^{[l-1]} + 2p - f}{s} + 1$$

**Transposed Convolution:** 

$$n_{W/H}^{[l]} = (n_{W/H}^{[l-1]} - 1)s - 2p + f$$

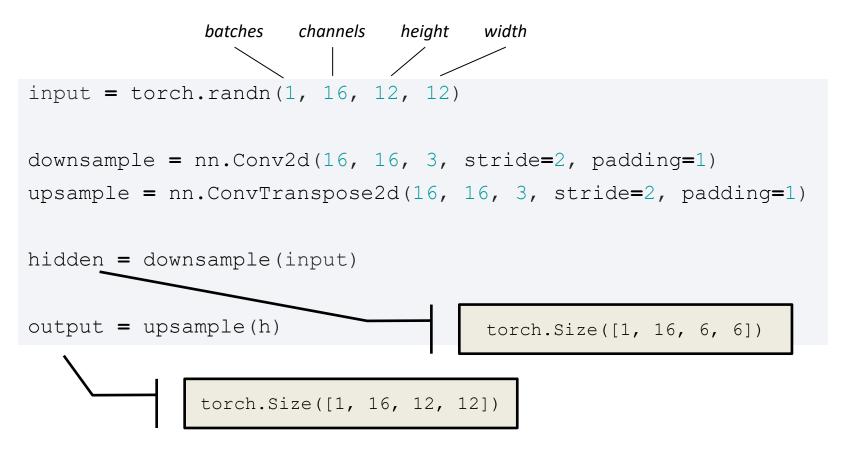
Filter size: j

Stride: s

# O PyTorch

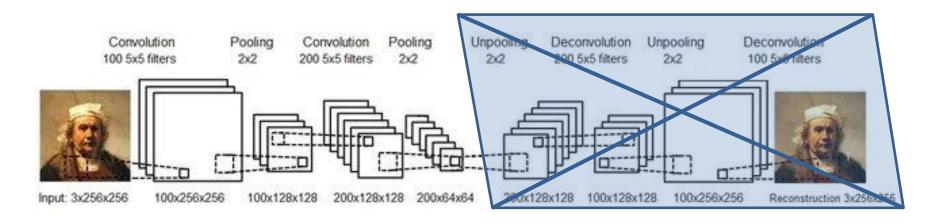
# **Transposed Convolutions**

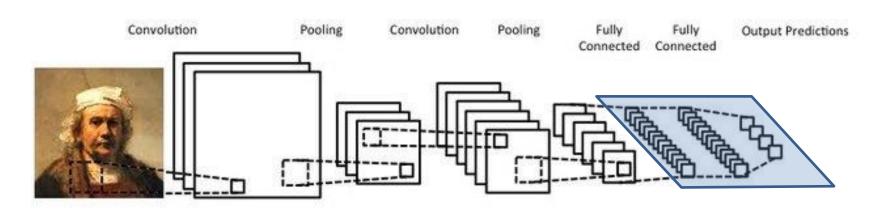
ConvTranspose2d() - see the documentation



### Autoencoders for weight initialisation

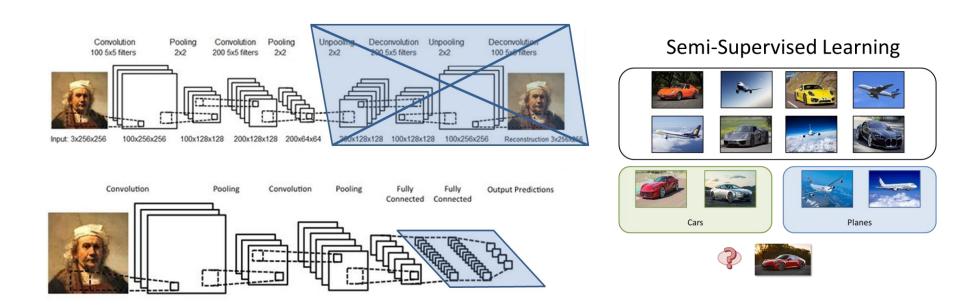
Makes sense if labeled training data is scarce, but unlabeled data is easy to get





### Autoencoders for weight initialisation

Makes sense if labeled training data is scarce, but unlabeled data is easy to get



### O PyTorch

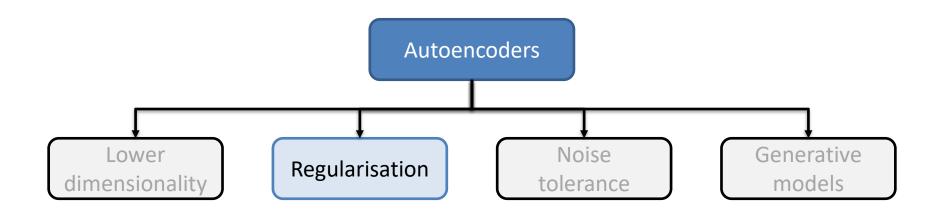
model = autoencoder().cuda()

criterion = nn.MSELoss()

### Convolutional AE

```
class autoencoder (nn. Module):
                                                       #Input: b, 1, 28, 28
    def init (self):
        super(autoencoder, self). init ()
        self.encoder = nn.Sequential(
            nn.Conv2d(1, 16, 3, stride=3, padding=1), # b, 16, 10, 10
            nn.ReLU(True), nn.MaxPool2d(2, stride=2), # b, 16, 5, 5
            nn.Conv2d(16, 8, 3, stride=2, padding=1), # b, 8, 3, 3
            nn.ReLU(True), nn.MaxPool2d(2, stride=1) # b, 8, 2, 2
        self.decoder = nn.Sequential(
            nn.ConvTranspose2d(8, 16, 3, stride=2),
                                                               #b,16,5,5
            nn.ReLU(True),
            nn.ConvTranspose2d(16, 8, 5, stride=3, padding=1), #b,8,15,15
            nn.ReLU(True),
            nn.ConvTranspose2d(8, 1, 2, stride=2, padding=1), \#b, 1, 28, 28
            nn.Tanh()
    def forward(self, x):
        z = self.encoder(x)
                                                   Note: This is a non
        x = self.decoder(z)
                                                   symmetric example
        return x
```

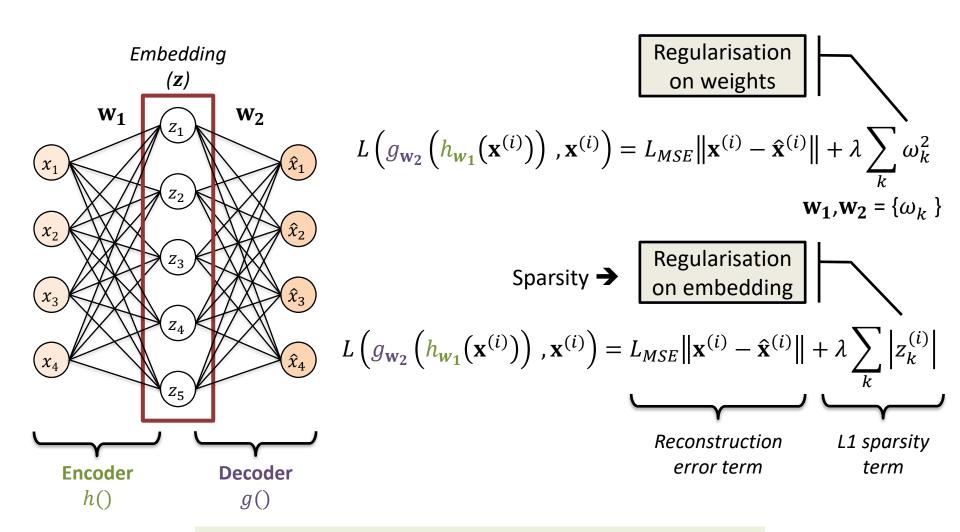
Convolution:  $n_{W/H}^{[l]} = \frac{n_{W/H}^{[l-1]} + 2p - f}{s} + 1$  Transposed Convolution:  $n_{W/H}^{[l]} = (n_{W/H}^{[l-1]} - 1)s - 2p + f$ 



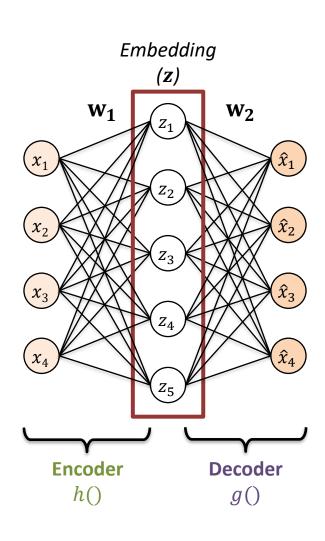
Regularisation – learning sparse / smooth embeddings

### REGULARISATION

# Regularise by enforcing sparsity



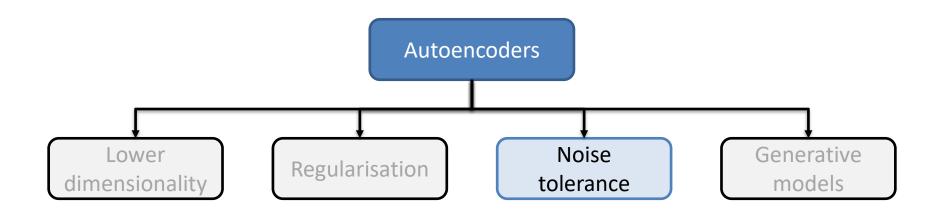
### Regularise by enforcing smoothness



Intuition: Points close to each other in input space should maintain that property in the embedding space

The "contractive" autoencoder encourages the derivatives of the embedding with respect to the input to be small, meaning that the representation of the input should be robust to small changes in the input

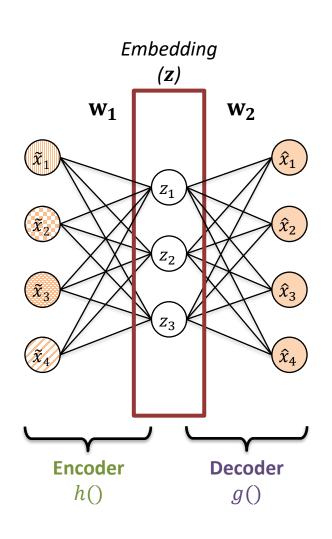
$$\begin{split} \|J_h(\mathbf{x})\|_F^2 &= \sum\nolimits_{j=1}^d \sum\nolimits_{i=1}^c \left(\frac{\partial h_i}{\partial x_j}(\mathbf{x})\right)^2 \\ \Omega_{CAE}(\mathbf{w}) &= \sum\nolimits_{x^i} \left\|J_h(\mathbf{x}^{(i)})\right\|_F^2 \\ L\left(g_{\mathbf{w}_2}\left(h_{\mathbf{w}_1}(\mathbf{x}^{(i)})\right), \mathbf{x}^{(i)}\right) &= L_{MSE} \left\|\mathbf{x}^{(i)} - \hat{\mathbf{x}}^{(i)}\right\| + \lambda \Omega_{CAE}(\mathbf{w}_1) \end{split}$$



Introduce a small change in the input and learn to undo it

### **NOISE TOLERANCE**

### **Denoising Autoencoders**



Intuition: learn to generate robust features from inputs by reconstructing partially destroyed samples

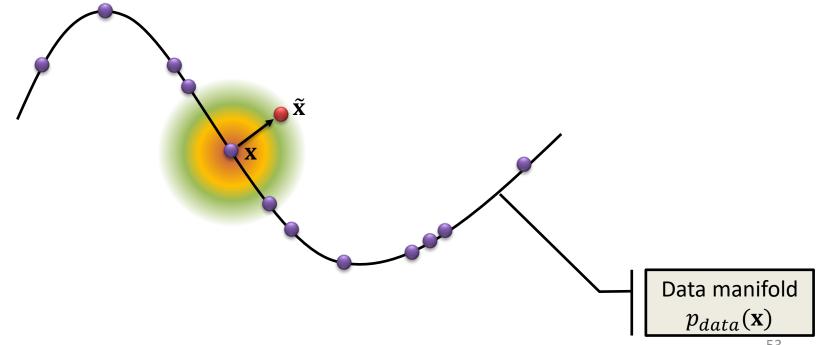
For every input x, we apply a corrupting function  $C(\cdot)$  to create noisy version:  $\tilde{\mathbf{x}} = C(\mathbf{x})$ 

$$L\left(g_{\mathbf{w}_{2}}\left(h_{\mathbf{w}_{1}}\left(\tilde{\mathbf{x}}^{(i)}\right)\right),\mathbf{x}^{(i)}\right) = L_{MSE} \|\mathbf{x}^{(i)} - \hat{\mathbf{x}}^{(i)}\|$$

$$\tilde{\mathbf{x}} = C(\mathbf{x})$$

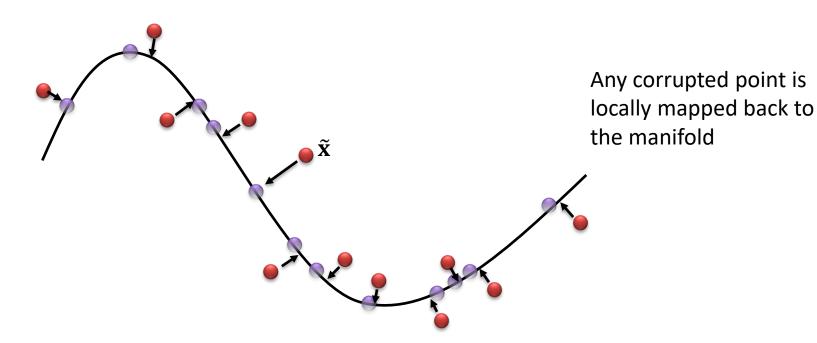
# Learning the manifold

The corrupting function  $C(\cdot)$  can corrupt in any direction. autoencoder must learn the "location" of data manifold and its distribution  $p_{data}(\mathbf{x})$ 



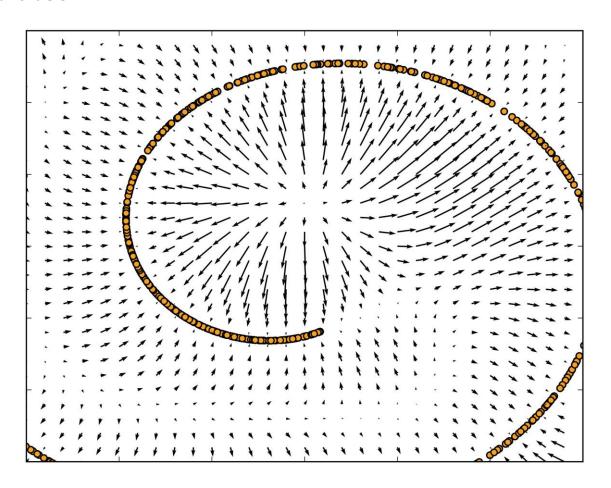
## Learning the manifold

The corrupting function  $C(\cdot)$  can corrupt in any direction. autoencoder must learn the "location" of data manifold and its distribution  $p_{data}(\mathbf{x})$ 

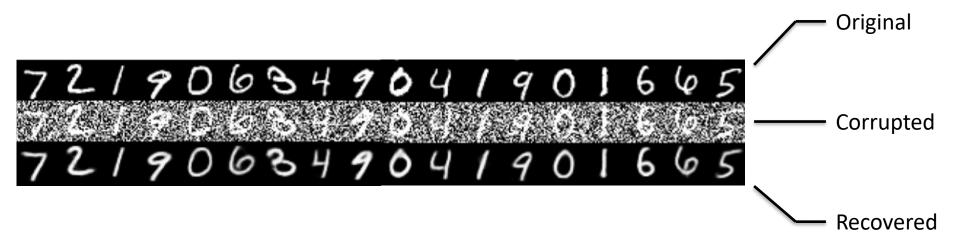


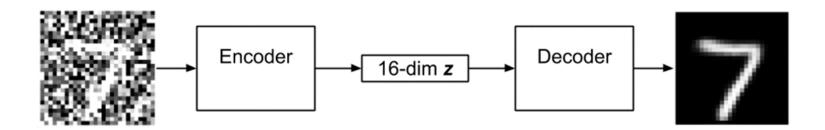
# Learning the manifold

2D vector field around a 1D curved manifold where the data concentrates



# **Denoising Example**

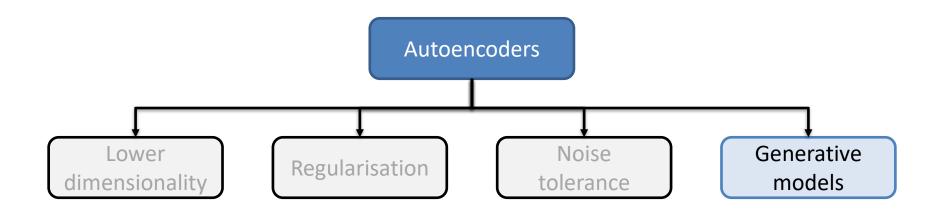




# Denoising examples



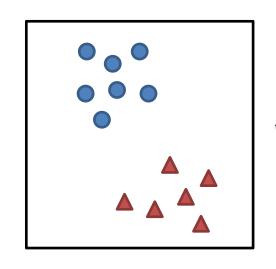


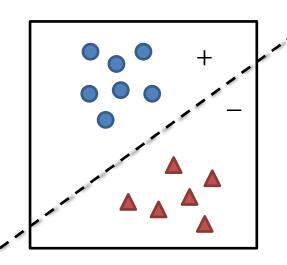


Generative models

### **VARIATIONAL AUTOENCODERS**

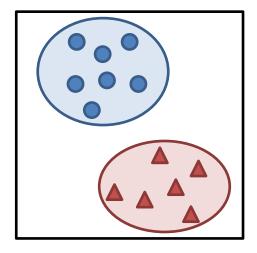
### Discriminative and Generative Models





#### **Discriminative models**

describe the decision surface; we can tell if a new point is on one side or another

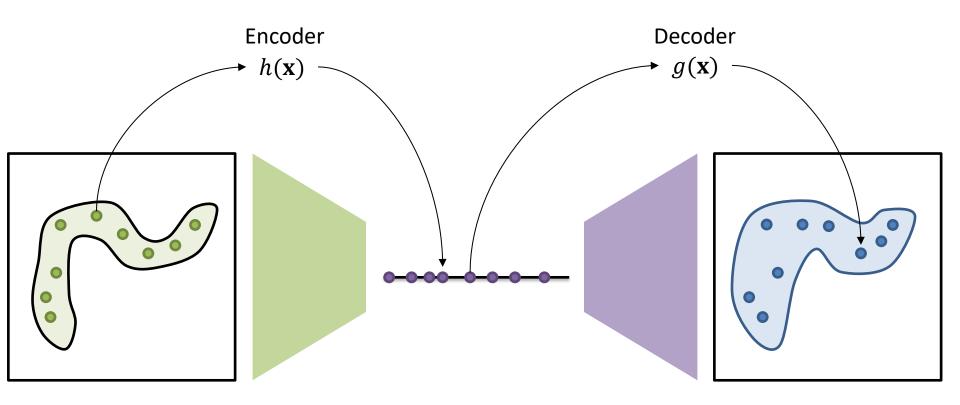


#### **Generative models**

describe the data distribution. We can ask which distribution a new point is most probable to come from

And we can use the learnt distributions to generate new data!

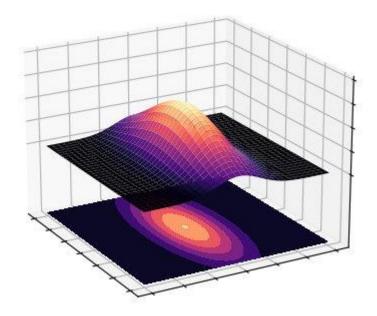
### What do autoencoders model?



Let's rethink the underlying idea of autoencoders. Instead of seeing the encoder and decoder as functions that map points between spaces, we can see them as probability distributions

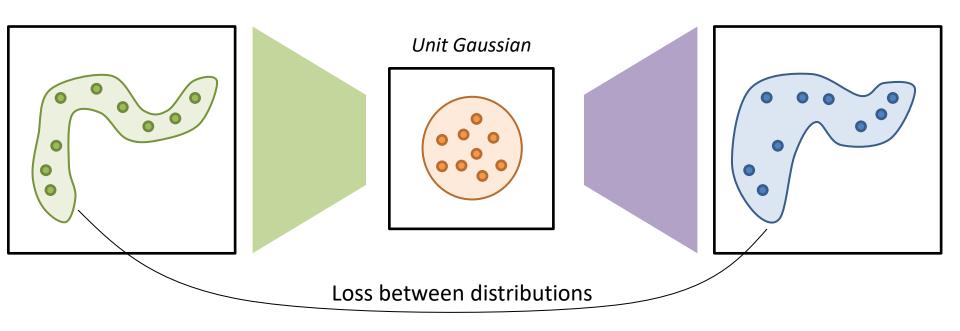
# Generating new data

Which is the probability of a pixel to be 'on' on an image representing number '1'



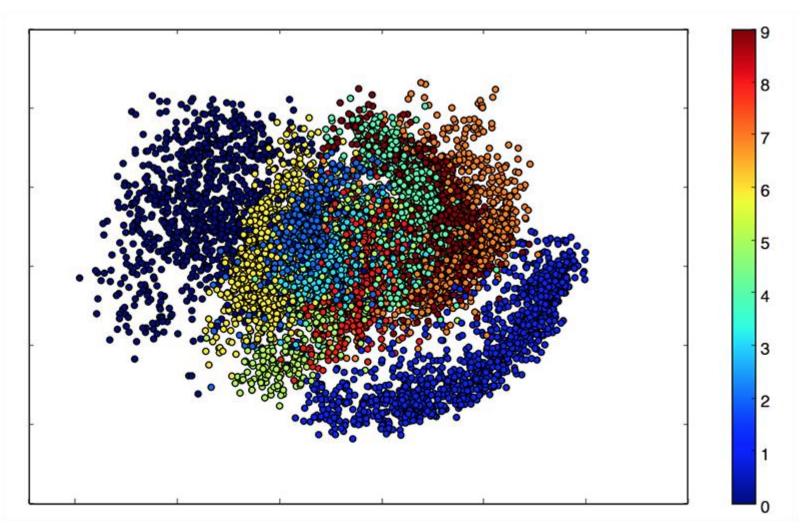
## Generating new data

Since we do not know the data distribution in the original space, we cannot directly generate new data

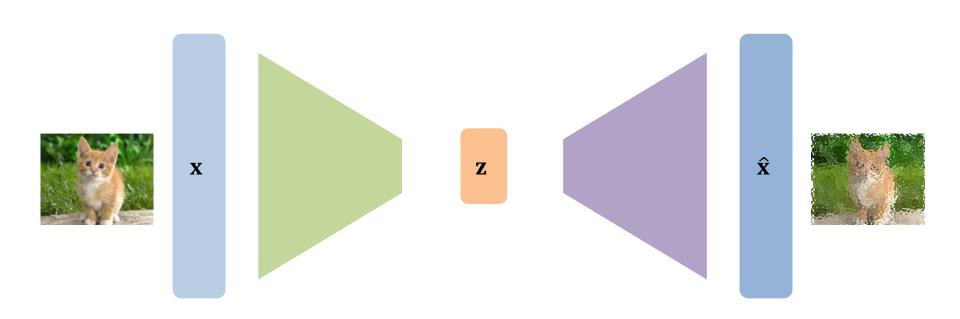


BUT, if we manage to map whatever distribution we have into a known distribution we know how to sample from, then we could use our generator to generate new data

# Unit Gaussian Embedding of MNIST data



### Traditional Autoencoder

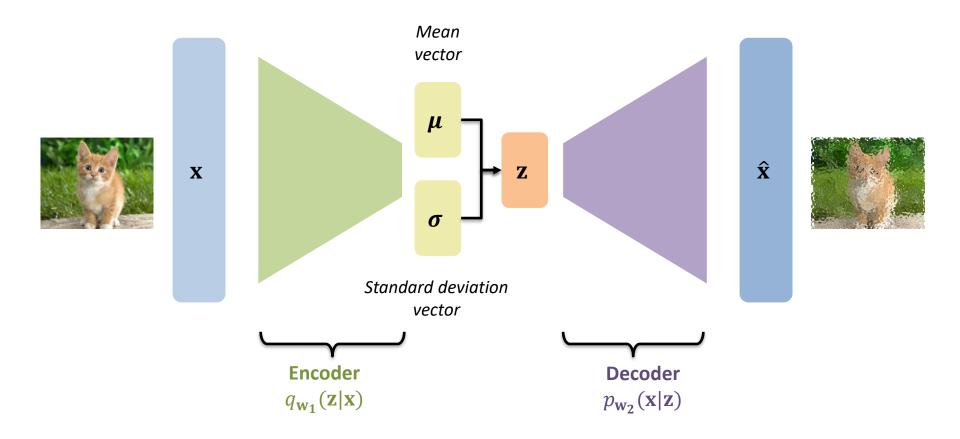


### Generative Autoencoders

- Generative models learn a distribution in order to be able to draw new samples from, different from those observed
- AEs can generally reconstruct encoded data, but are not necessarily able to build meaningful outputs from arbitrary encodings
- Variational and adversarial AEs learn a model of the data from which new instances can be generated

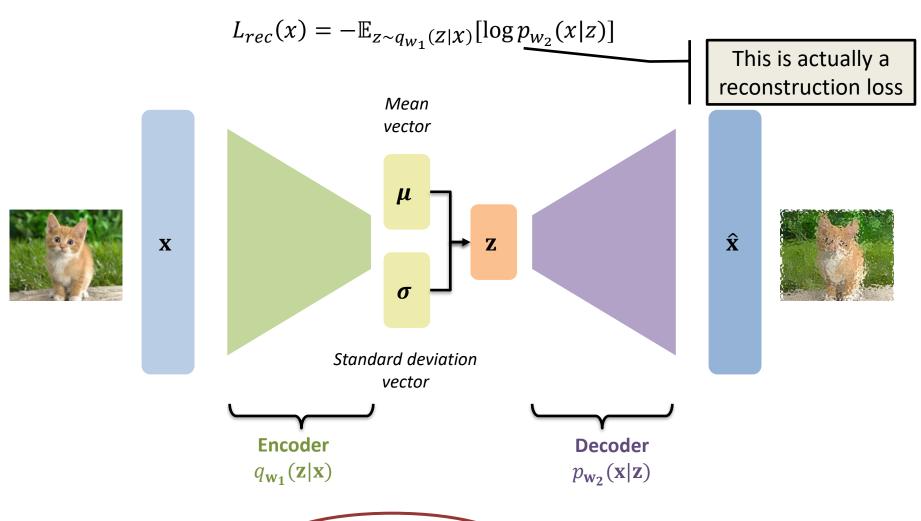
# Variational Autoencoders (VAE)

Input  $\rightarrow$  encode to statistics vectors  $\rightarrow$  sample a latent vector  $\rightarrow$  decode for reconstruction

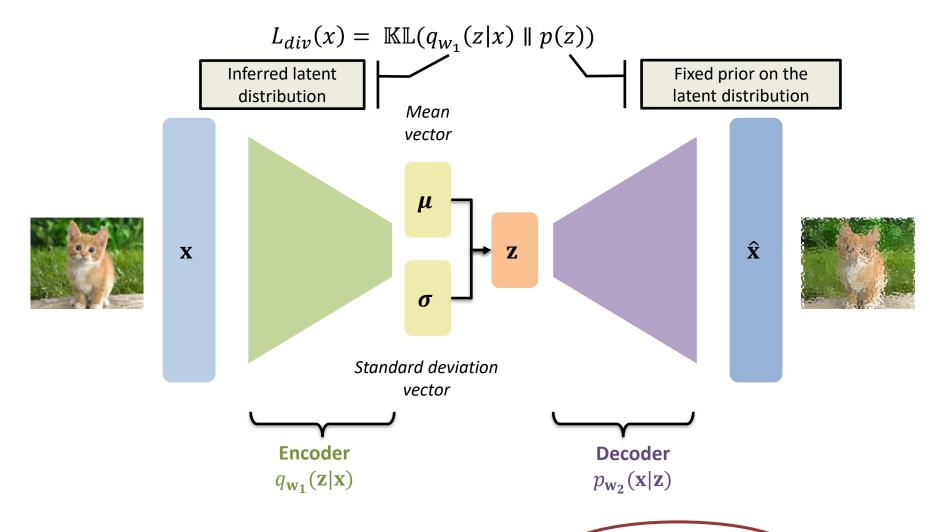


$$L(w_1, w_2, x) = (reconstruction \ loss) + (regularization \ term)$$

### Variational Autoencoders (VAE)

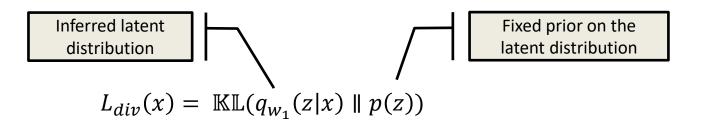


### Variational Autoencoders (VAE)

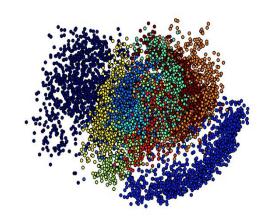


 $L(w_1, w_2, x) = (reconstruction loss) + (regularization term)$ 

### Prior on the latent distribution



$$L_{div}(x) = -\frac{1}{2} \sum_{j=0}^{k-1} (\sigma_j + \mu_j^2 - 1 - \log \sigma_j)$$

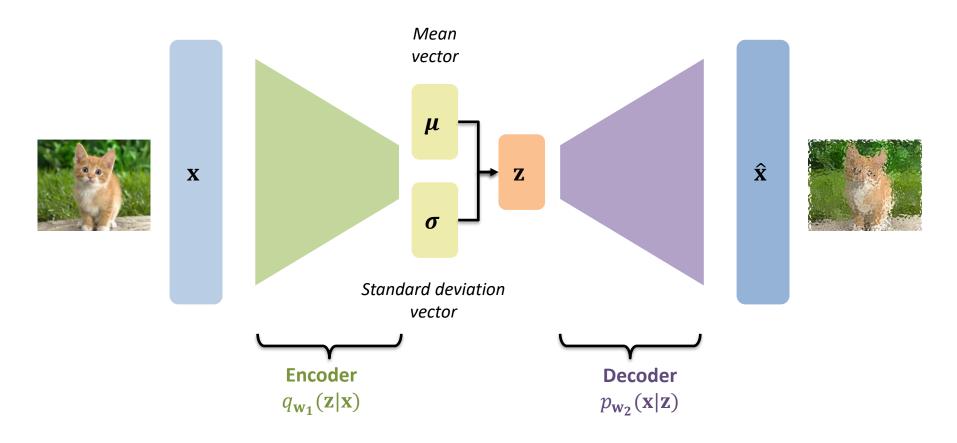


Common choice of prior – Normal Gaussian:

$$p(z) = N(\mu = 0, \sigma^2 = 1)$$

# Backpropagating

How can we backpropagate through the sampling process?



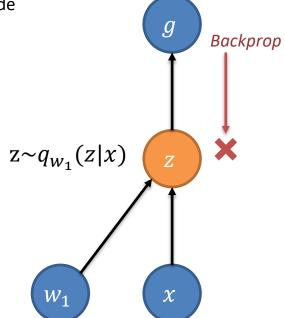
 $L(w_1, w_2, x) = (reconstruction loss) + (regularization term)$ 

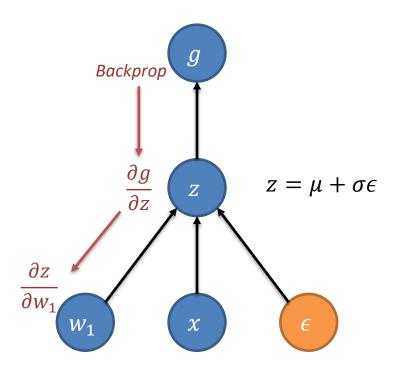
### Reparametrisation trick

Instead of thinking about z as a sample from a gaussian  $z \sim N(\mu, \sigma)$  think of it as the sum of the  $\mu$  and a fixed vector  $\sigma$  scaled by a random constant  $\epsilon$ 

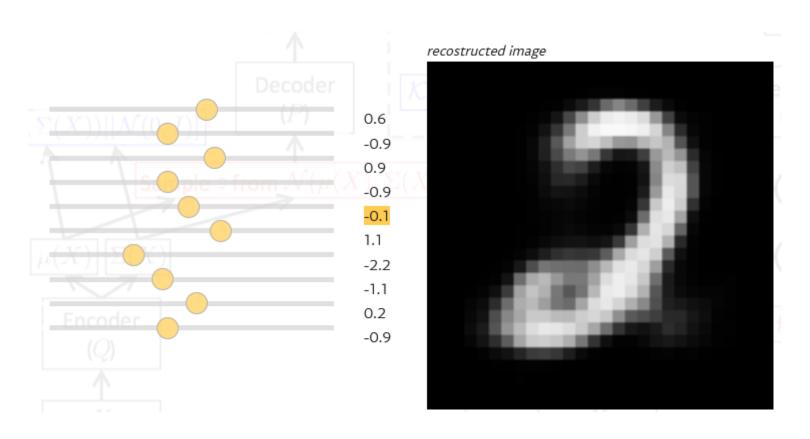
Deterministic node

Stochastic node





### Variational Autoencoder



https://www.siarez.com/projects/variational-autoencoder

### Autoencoders: standard

```
class StandardAE(nn.Module):
  def init (self):
       super(VAE, self). init ()
       self.fc1 = nn.Linear(784, 400)
       self.fc21 = nn.Linear(400, 20)
       self.fc3 = nn.Linear(20, 400)
       self.fc4 = nn.Linear(400, 784)
  def encode(self, x):
      h1 = F.relu(self.fc1(x))
       return self.fc21(h1)
  def decode(self, z):
      h3 = F.relu(self.fc3(z))
       return F.sigmoid(self.fc4(h3))
  def forward(self, x):
                  = self.encode(x)
       return self.decode(z)
```

### Autoencoders: code – VAE

```
class VAE(nn.Module):
  def init (self):
       super(VAE, self). init ()
       self.fc1 = nn.Linear(784, 400)
       self.fc21 = nn.Linear(400, 20)
       self.fc22 = nn.Linear(400, 20)
       self.fc3 = nn.Linear(20, 400)
       self.fc4 = nn.Linear(400, 784)
  def encode(self, x):
      h1 = F.relu(self.fc1(x))
       return self.fc21(h1), self.fc22(h1)
  def decode(self, z):
      h3 = F.relu(self.fc3(z))
       return F.sigmoid(self.fc4(h3))
  def forward(self, x):
      mu, logvar = self.encode(x)
       return self.decode(z), mu, logvar
```

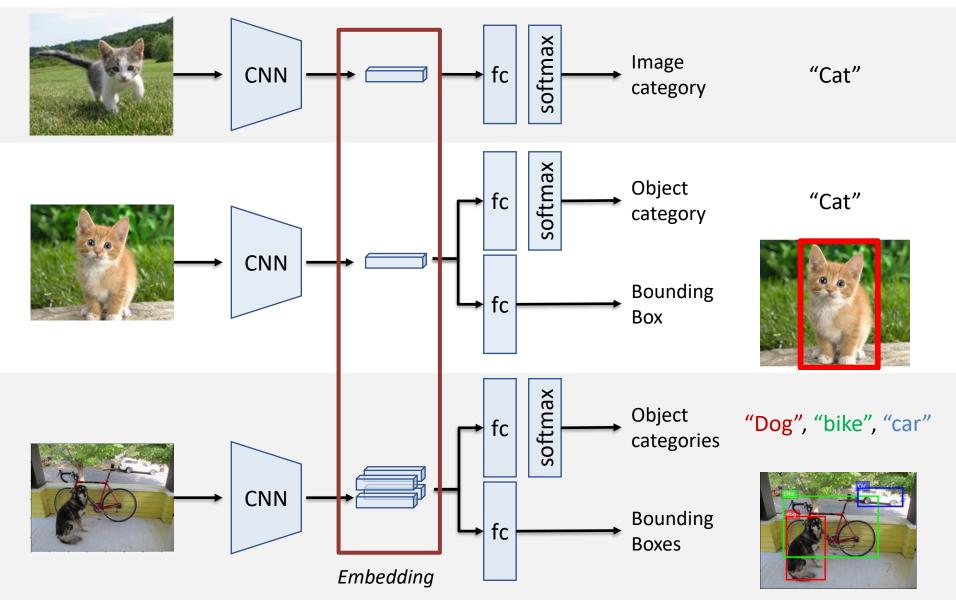
### Autoencoders: code – VAE

```
class VAE (nn.Module):
   def init (self):
       super(VAE, self). init ()
       self.fc1 = nn.Linear(784, 400)
       self.fc21 = nn.Linear(400, 20)
       self.fc22 = nn.Linear(400, 20)
       self.fc3 = nn.Linear(20, 400)
       self.fc4 = nn.Linear(400, 784)
   def encode(self, x):
       h1 = F.relu(self.fc1(x))
       return self.fc21(h1), self.fc22(h1)
   def reparametrize(self, mu, logvar):
       std = logvar.mul(0.5).exp()
       eps = torch.cuda.FloatTensor(std.size()).normal ()
       eps = Variable(eps)
       return eps.mul(std).add_(mu) z = \mu + \sigma \epsilon
                                                def loss function (recon x, x, mu, logvar):
   def decode(self, z):
                                                    BCE = F.binary cross entropy(recon x,
       h3 = F.relu(self.fc3(z))
                                                                      x.view(-1, 784), reduction='sum')
       return F.sigmoid(self.fc4(h3))
                                                    # see Appendix B from VAE paper:
   def forward(self, x):
                                                    # Kingma and Welling. Auto-Encoding Variational Bayes
       mu, logvar = self.encode(x)
                                                    # https://arxiv.org/abs/1312.6114
       z = self.reparametrize(mu, logvar)
                                                    \# 0.5 * sum(1 + log(sigma^2) - mu^2 - sigma^2)
       return self.decode(z), mu, logvar
                                                    KLD = -0.5 * torch.sum(1 + logvar - mu.pow(2))
                                                                                 - logvar.exp())
```

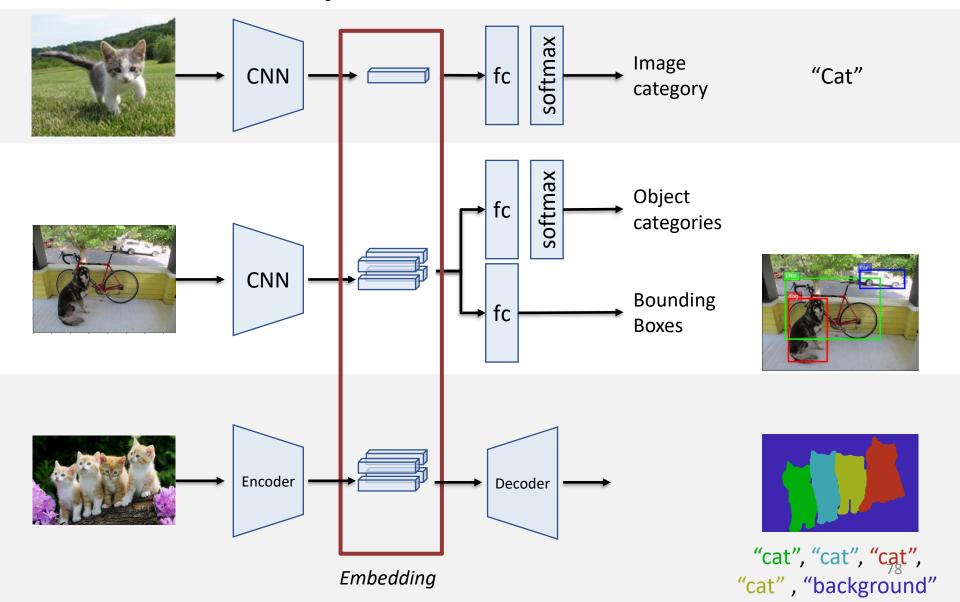
**Encoder-Decoder Architectures** 

### **EXTENDING THE CONCEPT**

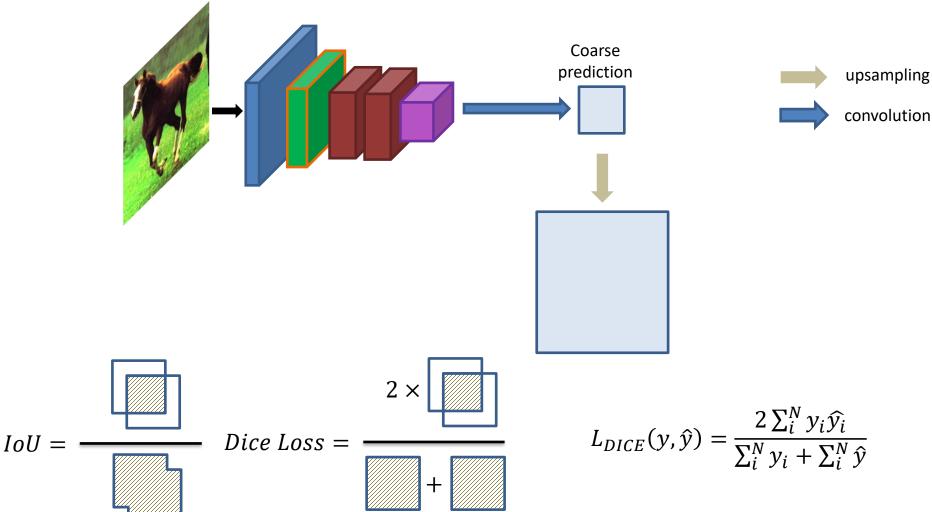
# **Computer Vision Tasks**



## **Computer Vision Tasks**



## Autoencoder for image segmentation

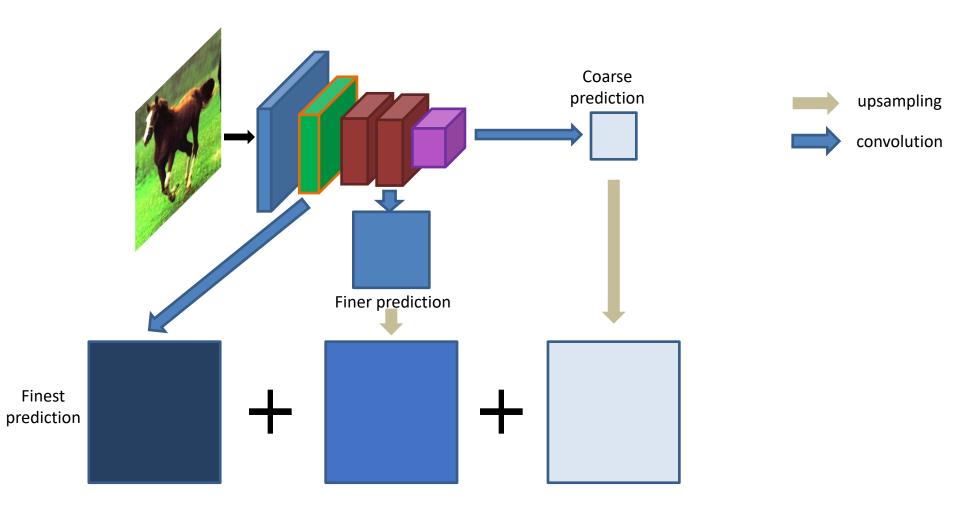


# Semantic segmentation using convolutional networks



Very coarse segmentation

# Solution: Skip connections

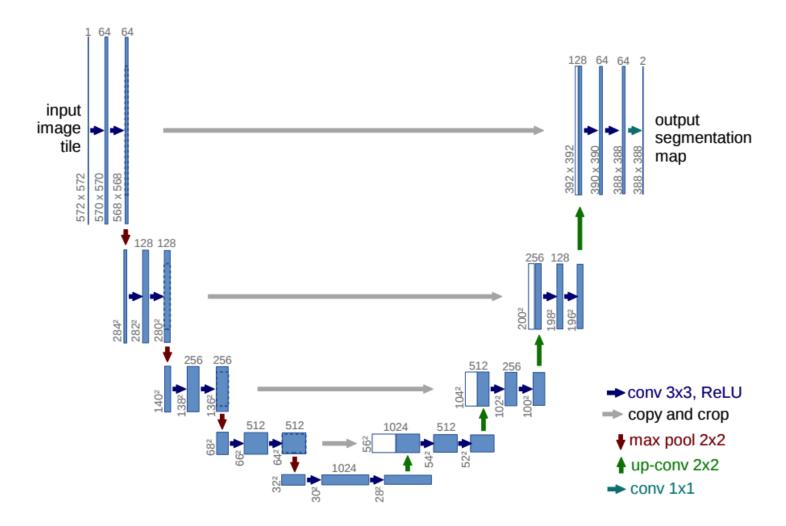


## Skip connections



Details are still a problem

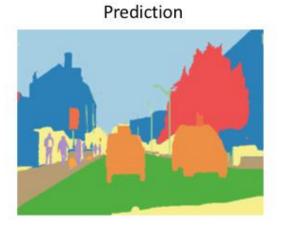
## **U-Net**



## **U-Net**

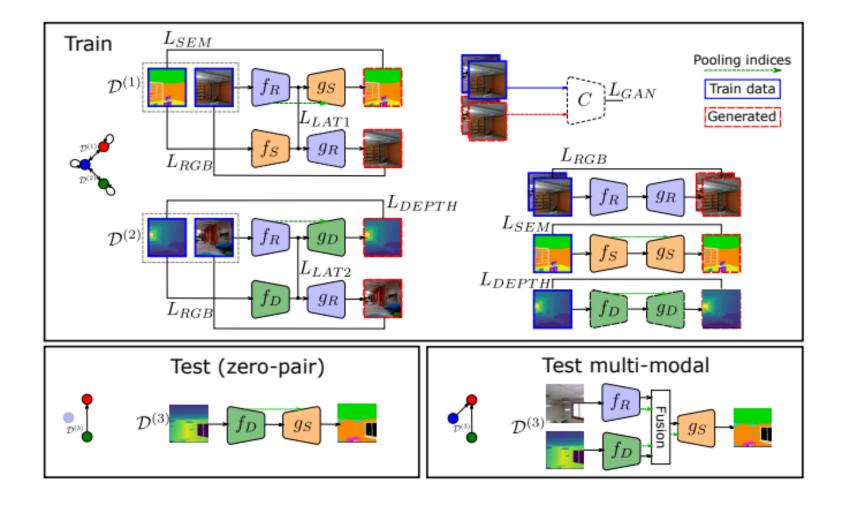
Input

Ground truth



FC-DenseNet103 model on UNET

# Mixing and Matching encoders and decoders

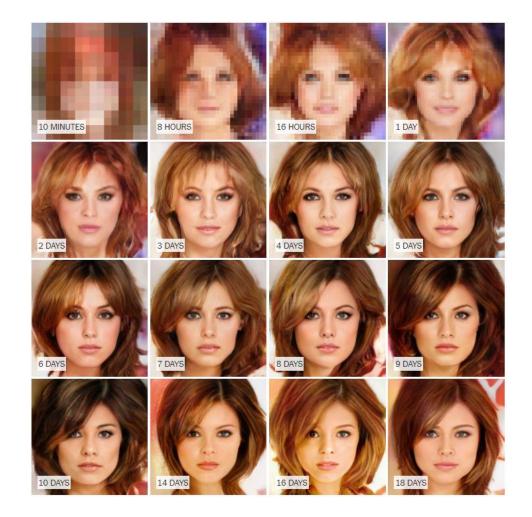


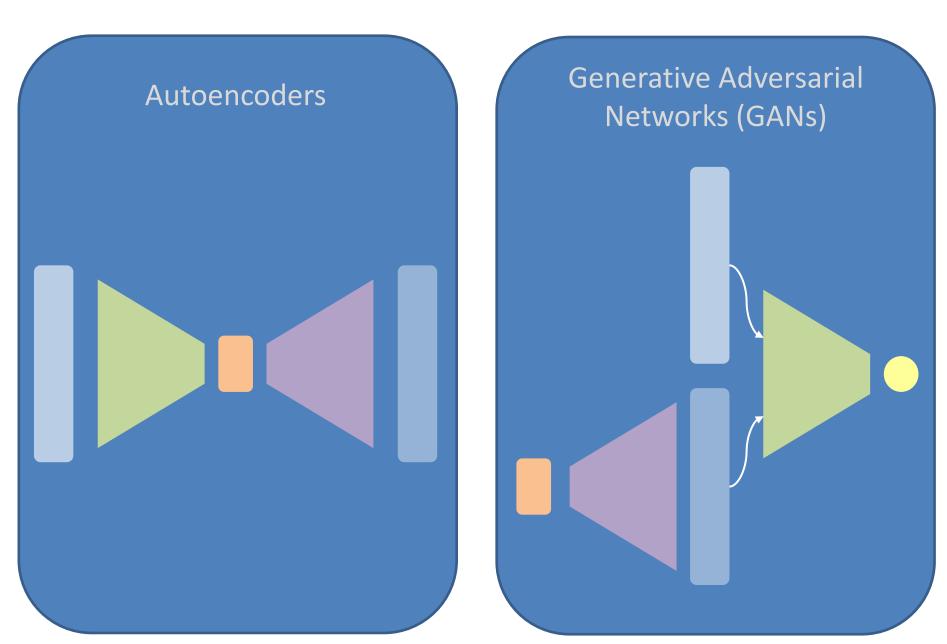
# GENERATIVE ADVERSARIAL NETWORKS

## Real or Fake?









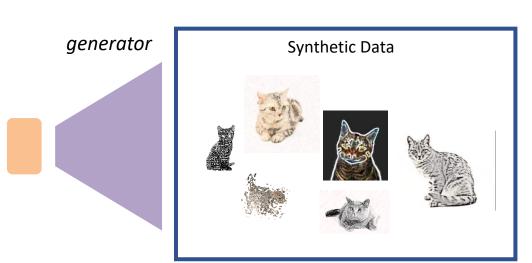
#### **GAN:** Generative Adversarial Networks

#### Two NNs competing against each other

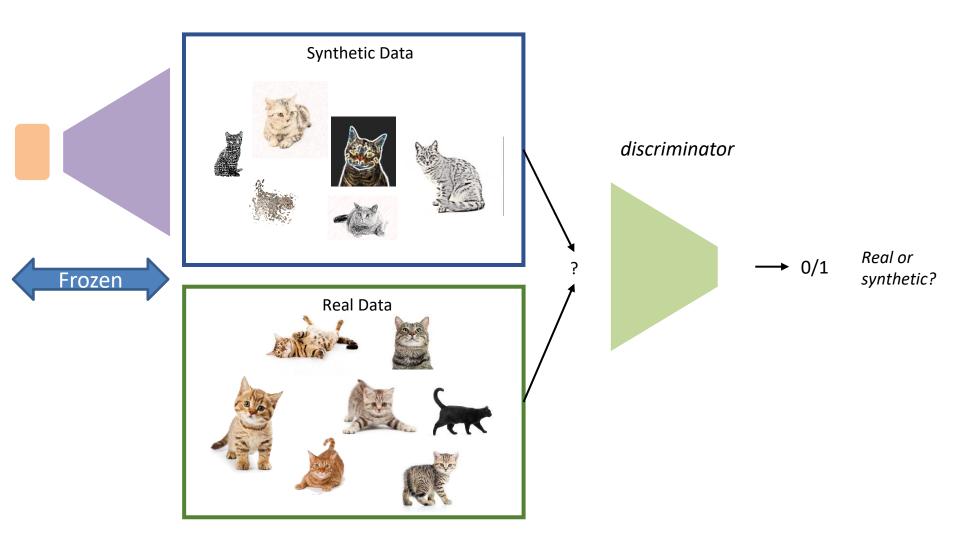
- The generator NN learns to generate plausible data.
   The generated instances become negative training examples for the discriminator.
- The **discriminator** NN learns to distinguish the generator's fake data from real data. The discriminator penalizes the generator for producing implausible results.



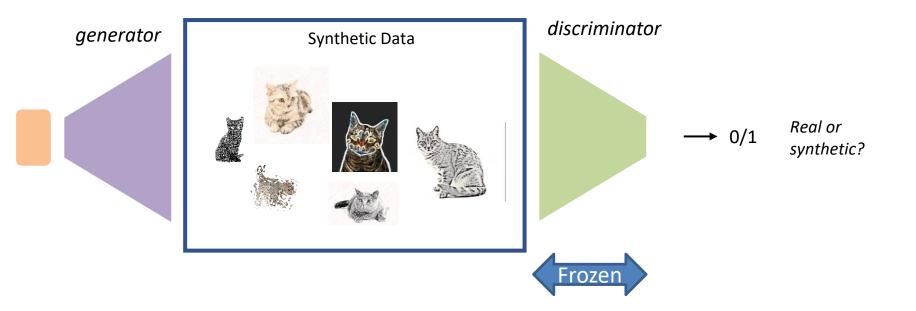
## **GAN Process**



## **GAN Process**



## **GAN Process**



## Generative Adversarial Networks



The OG

GAN

Deep

Convolutional

**GAN** 





GAN





Progressively Growing GAN



Style-based **GAN** 

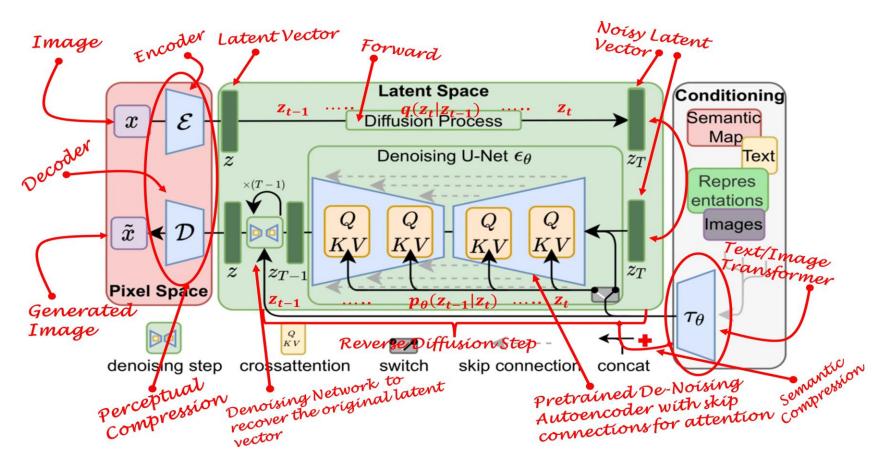


2020 **Improved** Style-based **GAN** 

### The GAN zoo

https://github.com/hindupuravinash/the-gan-zoo

## And now? Stable Difussion Models



## Resources (I)



I. Goodfellow, Y. Bengio, A. Courville, "Deep Learning", MIT Press, 2016

http://www.deeplearningbook.org/



C. Bishop, "Pattern Recognition and Machine Learning", Springer, 2006

http://research.microsoft.com/enus/um/people/cmbishop/prml/index.htm



D. MacKay, "Information Theory, Inference and Learning Algorithms", Cambridge University Press, 2003
<a href="http://www.inference.phy.cam.ac.uk/mackay/">http://www.inference.phy.cam.ac.uk/mackay/</a>



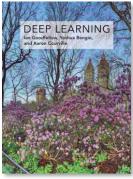
R.O. Duda, P.E. Hart, D.G. Stork, "Pattern Classification", Wiley & Sons, 2000

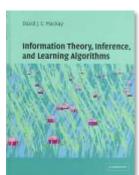
http://books.google.com/books/about/Pattern Classificati on.html?id=Br33IRC3PkQC



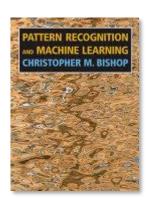
J. Winn, C. Bishop, "Model-Based Machine Learning", early access

http://mbmlbook.com/











### **Further Info**

- Many of the slides of these lectures have been adapted from various highly recommended online lectures and courses:
  - Andrew Ng's Machine Learning Course, Coursera https://www.coursera.org/course/ml
  - Andrew Ng's Deep Learning Specialization, Coursera <a href="https://www.coursera.org/specializations/deep-learning">https://www.coursera.org/specializations/deep-learning</a>
  - Victor Lavrenko's Machine Learning Course
     <a href="https://www.youtube.com/channel/UCs7alOMRnxhzfKAJ4JjZ7Wg">https://www.youtube.com/channel/UCs7alOMRnxhzfKAJ4JjZ7Wg</a>
  - Fei Fei Li and Andrej Karpathy's Convolutional Neural Networks for Visual Recognition http://cs231n.stanford.edu/
  - Geoff Hinton's Neural Networks for Machine Learning, (ex Coursera)
     <a href="https://www.youtube.com/playlist?list=PLiPvV5TNogxKKwvKb1RKwkq2hm7ZvpHz0">https://www.youtube.com/playlist?list=PLiPvV5TNogxKKwvKb1RKwkq2hm7ZvpHz0</a>
  - Luis Serrano's introductory videos
     <a href="https://www.youtube.com/channel/UCgBncpylJ1kiVaPyP-PZauQ">https://www.youtube.com/channel/UCgBncpylJ1kiVaPyP-PZauQ</a>
  - Michael Nielsen's Neural Networks and Deep Learning <a href="http://neuralnetworksanddeeplearning.com/">http://neuralnetworksanddeeplearning.com/</a>
  - David Charte et al. A practical tutorial on autoencoders for nonlinear feature fusion: Taxonomy, models, software and guidelines <a href="https://arxiv.org/abs/1801.01586">https://arxiv.org/abs/1801.01586</a>