# Técnicas de lA para Biologia

# 5 - Autoencoders

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#### Autoencoders

### **Summary**

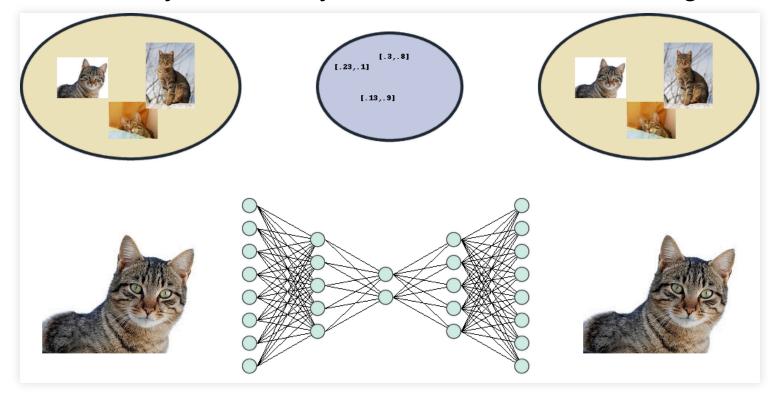
- What are Autoencoders?
- Different restrictions on encoding
- Undercompleteness
- Regularization
- Sparsity
- Noise reconstruction
- Applications

## Autoencoders

# What are autoencoders?

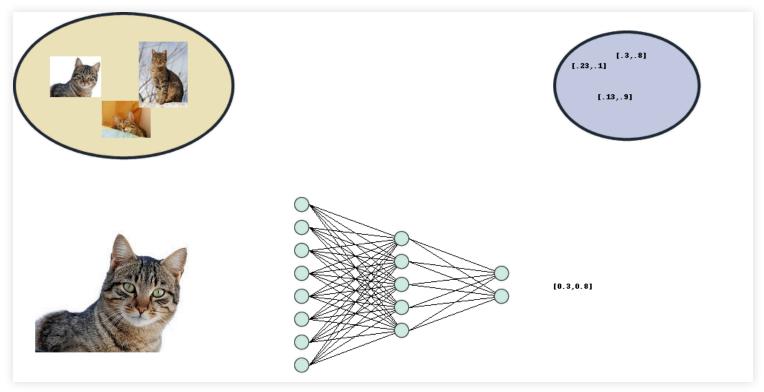
### **Network trained to output the input (unsupervised)**

■ In the hidden layers, one layer learns a **code** describing the input



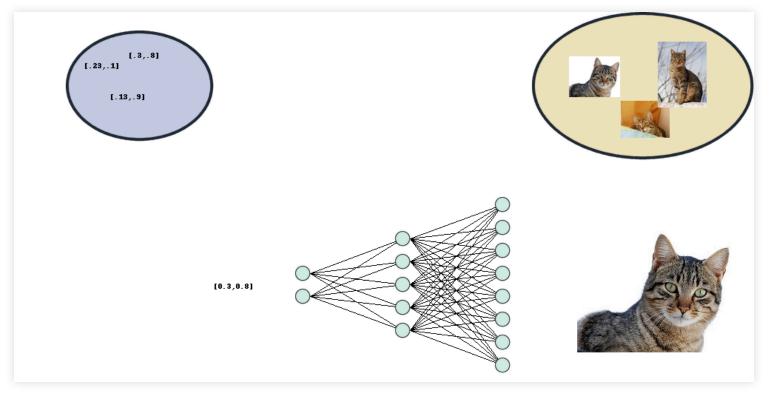
### **Network trained to output the input (unsupervised)**

■ The encoder maps from input to latent space



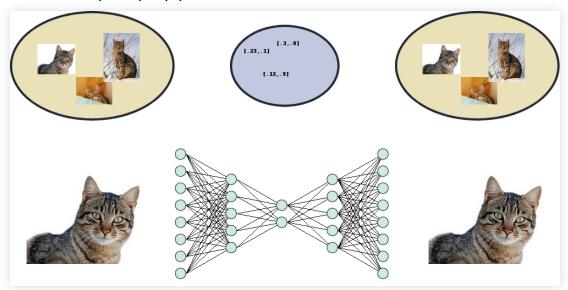
### **Network trained to output the input (unsupervised)**

■ The decoder maps from **latent space** back to input space



#### **Network trained to output the input (unsupervised)**

- lacksquare Encoder, h=f(x), and decoder, x=g(h)
- No need for labels, since the target is the input
- Why learn x = g(f(x))?



Cat images: Joaquim Alves Gaspar CC-SA

#### **Network trained to output the input (unsupervised)**

- lacksquare Encoder, h=f(x), and decoder, x=g(h)
- Why learn x = g(f(x))?
- Latent representation can have advantages
- Lower dimension
- Capture structure in the data
- Data generation

#### **Network trained to output the input (unsupervised)**

- lacksquare Encoder, h=f(x), and decoder, x=g(h)
- Autoencoders are (usually) feedfoward networks
- Can be trained with the same algorithms, such as backpropagation
- $\blacksquare$  But since the target is x, they are unsupervised learners
- Need some "bottleneck" to force a useful representation
- Otherwise just copies values

#### Autoencoders

# Different types of autoencoders

## **Undercomplete Autoencoders**

### Autoencoder is undercomplete if h is smaller than x

- Forces the network to learn reduced representation of input
- Trained by minimizing a loss function

$$L(x,g(f(x)))$$
 that penalizes the difference between  $x$  and  $g(f(x))$ 

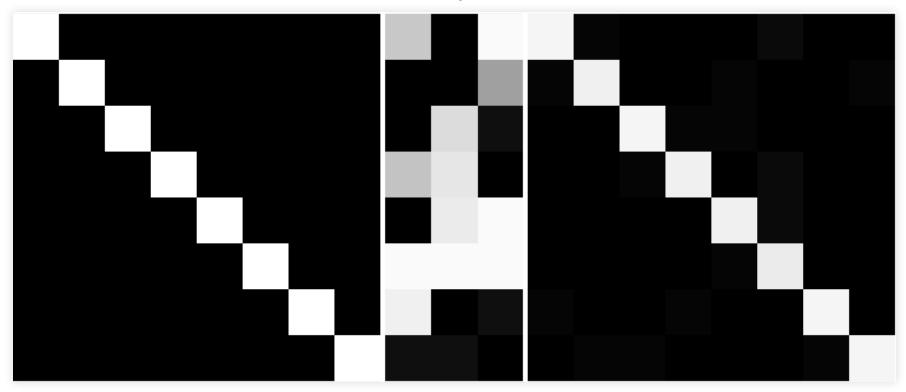
- If linear it is similar to PCA (without orthogonality constraint)
- With nonlinear transformations, an undercomplete autoencoder can learn more powerful representations
- However, we cannot overdo it
- With too much power, autoencoder can just index each training example and learn nothing useful:

$$f(x_i) = i, \quad g(i) = x_i$$

## Undercomplete Autoencoders

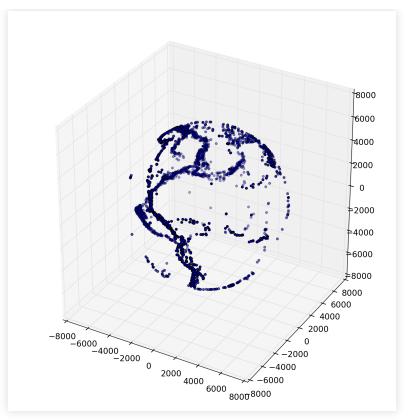
## Autoencoder is undercomplete if h is smaller than x

Mitchell's autoencoder, hidden layer of 3 neurons

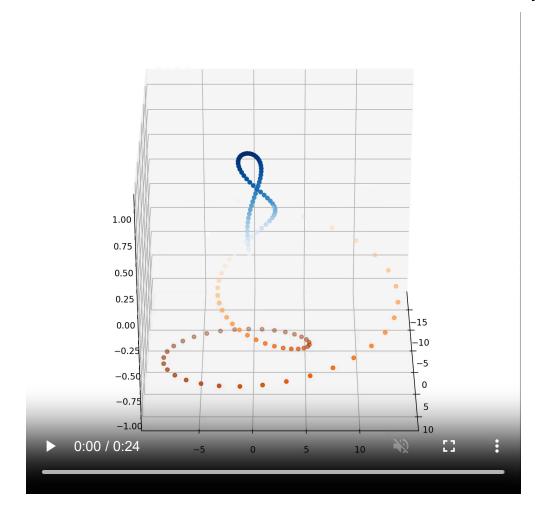


#### **Manifold**

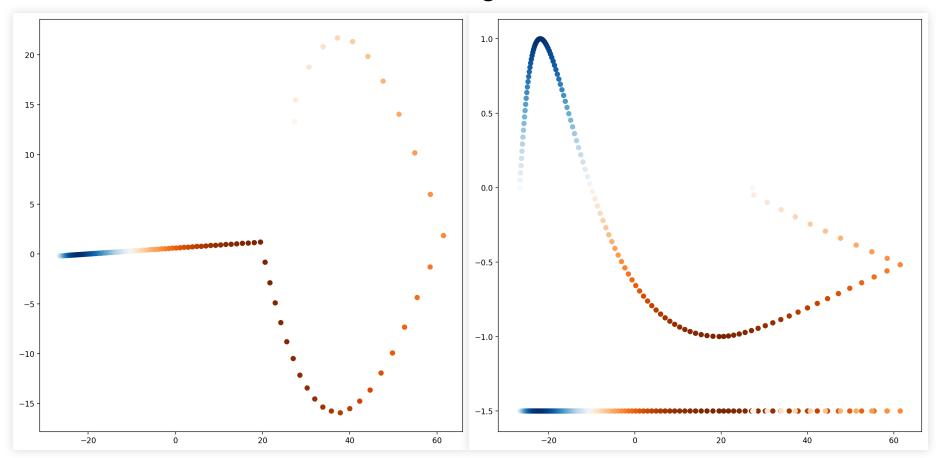
- A set of points such that the neighbourhood of each is homeomorphic to a euclidean space
  - Example: the surface of a sphere



Data may cover a lower dimension manifold of the space

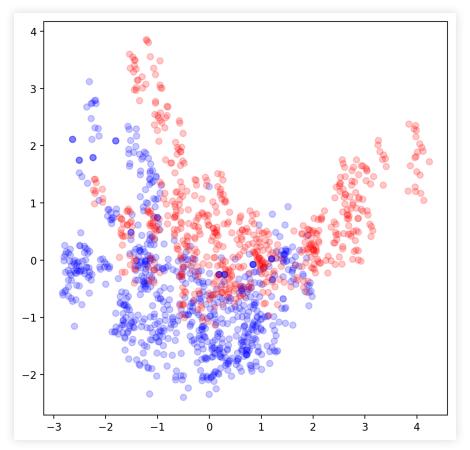


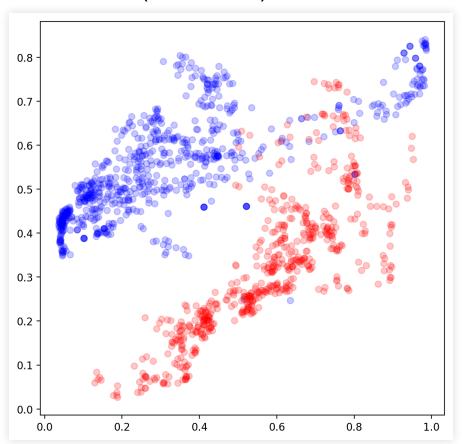
Learn lower dimension embeddings of data manifold



## Undercomplete Autoencoders

- Nonlinearity makes dimensionality reduction adapt to manifold
- PCA vs autoencoder 6,4,2,4,6, UCI banknote dataset (4 features)





#### Manifold learning with autoencoders

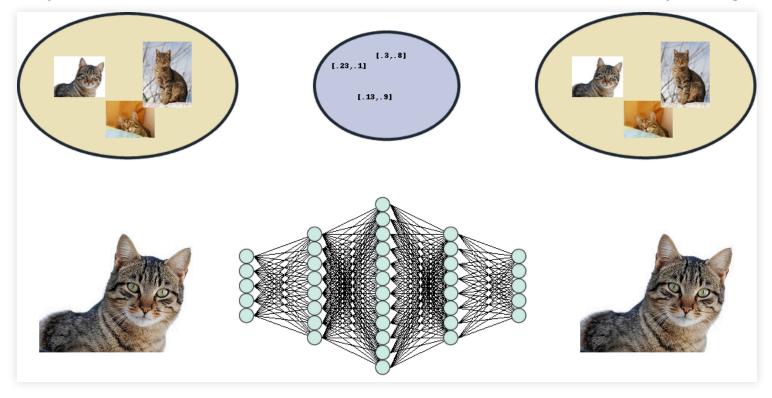
- This works because we force the network in two opposite ways:
- We demand the ability to reconstruct the input
- But we also constrain how the network can encode the examples
- Undercompleteness is just one way of doing this

#### Beware of overfitting.

- If the autoencoder is sufficiently powerful, it can reconstruct the training data accurately but lose generalization power
- In the extreme, all information about reconstructing the training set may be in the weights and the latent representation becomes useless

#### An overcomplete autoencoder has h larger than x

lacktriangle This, by itself, is a bad idea as h will not represent anything useful



### An overcomplete autoencoder has h larger than x

- But we can restrict h with regularization
- lacksquare This way the autoencoder also learns how restricted h should be

#### **Sparse Autoencoder**

- Force h to have few activations
- lacktriangle Example: we want the probability of  $h_i$  firing

$$\hat{p}_i = rac{1}{m} \sum_{j=1}^m h_i(x_j)$$

to be equal to p (the sparseness parameter)

#### **Sparse Autoencoder**

- Include in the loss function a penalization term
- Use the Kullback-Leibler divergence between Bernoulli variables as a regularization penalty

$$L(x,g(f(x))) + \lambda \sum_i \left(p\lograc{p}{\hat{p}_i} + (1-p)\lograc{1-p}{1-\hat{p}_i}
ight)$$

 Other options include L1 regularization applied to the activation of the neurons, L2, etc.

#### **Sparse Autoencoder**

Sparse autoencoders make neurons specialize

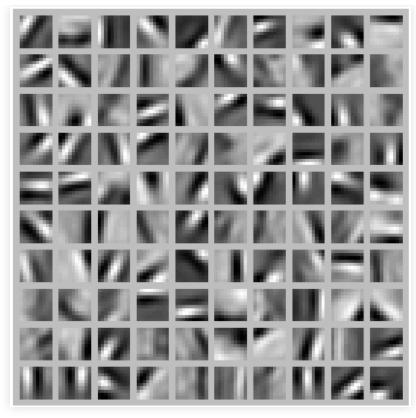
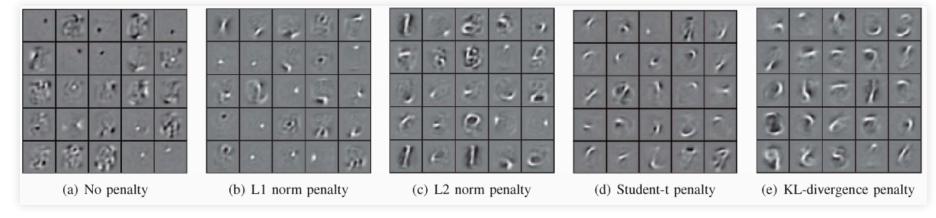


Image: Andrew Ng

- Trained on 10x10 images
- lacksquare 100 neurons on h
- Images (norm-bounded) that maximize activation

#### **Sparse Autoencoder**

- Sparse autoencoders trained on MNIST, different sparsity penalties
- (25 neurons in filter, images correspond to highest activation)



Niang et. al, Empirical Analysis of Different Sparse Penalties... IJCNN 2015,

#### **Denoising Autoencoders**

- We can force h to be learned with noisy inputs
- Output the original x from corrupted  $ilde{x}$ :  $L(x,g(f( ilde{x})))$

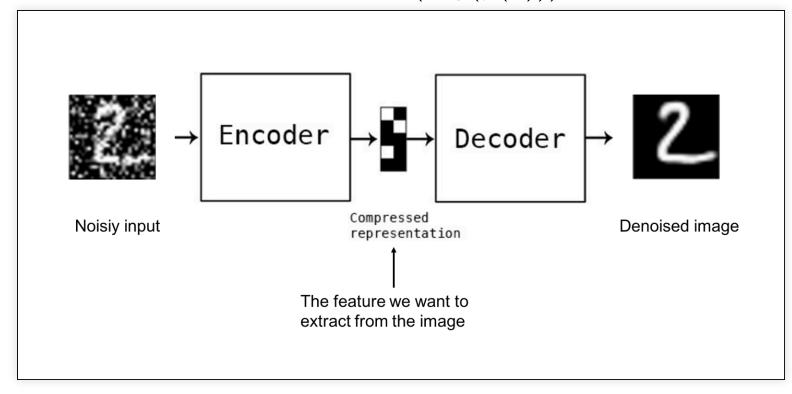


Image: Adil Baaj, Keras Tutorial on DAE

#### **Denoising Autoencoders**

- lacktriangle We can force h to be learned with noisy inputs
- Output the original x from corrupted  $ilde{x}$ :  $L(x,g(f( ilde{x})))$
- lacktriangle This forces the autoencoder to remove the noise by learning the underlying distribution of x
- Algorithm:
- Sample  $x_i$  from  ${\cal X}$
- Apply corruption  $C(\tilde{x_i} \mid x_i)$
- Train with  $(x, \tilde{x})$

#### Stochastic Autoencoders

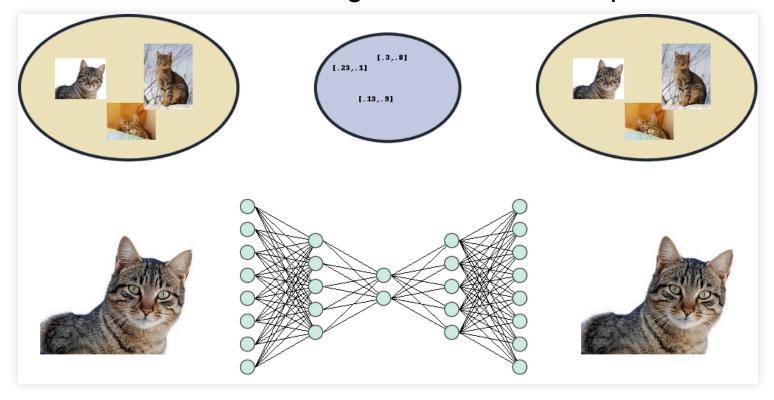
- We can also use autoencoders to learn probabilities
- Just like with other ANN (e.g. softmax classifier)
- lacksquare The decoder is modelling a conditional probability  $p_{decoder}(x\mid h)$
- ullet where h is given by the encoder part of the autoencoder
- The decoder output units can be chosen as before:
- Linear for estimating the mean of Gaussian distributions
- Sigmoid for Bernoulli (binary)
- Softmax for discrete categories
- We can think of encoder and decoder as modelling conditional probabilities

$$p_{encoder}(h \mid x) \qquad p_{decoder}(x \mid h)$$

## Autoencoders

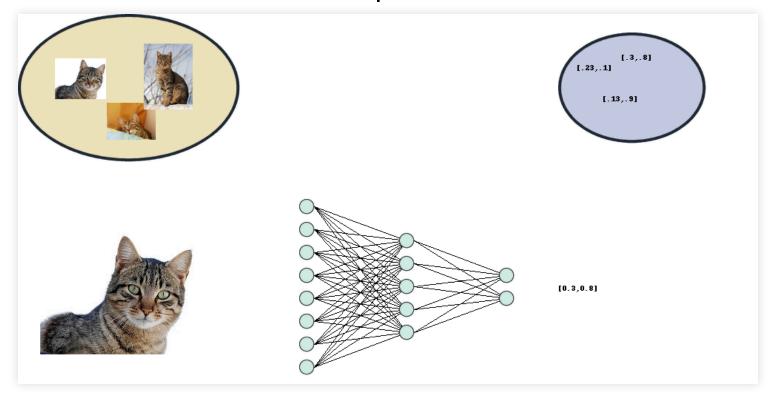
# **Generating Data**

Can we use autoencoders to generate new examples?

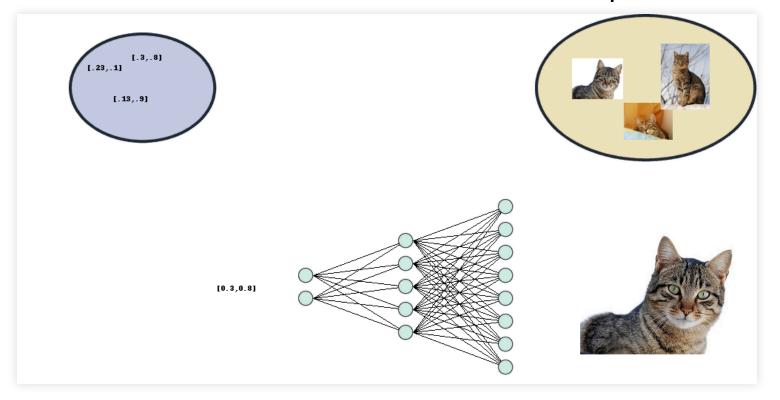


Cat images: Joaquim Alves Gaspar CC-SA

Autoencoders create a latent representation from the data



And then decode to recreate the data from this representation



Cat images: Joaquim Alves Gaspar CC-SA

Can we use the decoder to generate new examples?

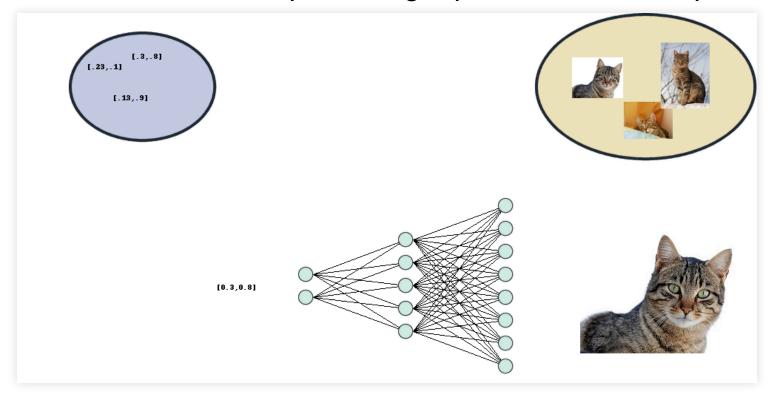
#### Discriminative vs Generative

- lacksquare A discriminative model tries to approximate a function  $p(y \mid x)$
- E.g. Logistic regression or softmax ANN predict the probability of each class given the features
- lacksquare A generative model approximates p(x,y) and then finds  $p(y\mid x)$ :  $p(x,y)=p(y\mid x)p(x)$
- ullet This is generative because, knowing p(x,y), we can sample from the distribution

#### With autoencoders

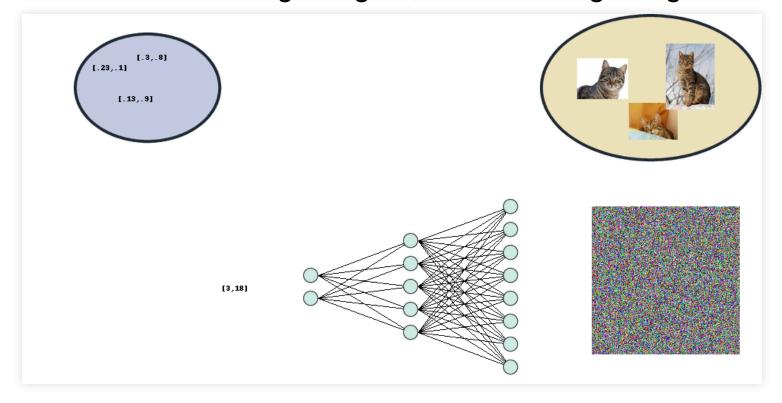
• We decode from h, so we need to find its distribution in order to generate examples from  $p(h,y)=p(y\mid h)p(h)$ 

Intuition: we need to sample the right part of the latent space



Cat images: Joaquim Alves Gaspar CC-SA

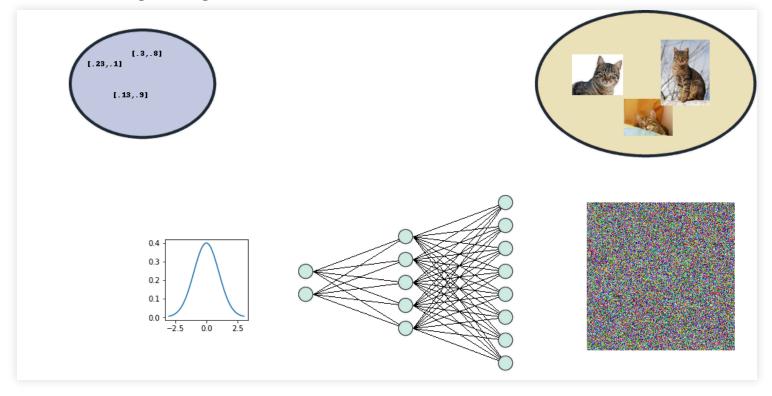
Intuition: if outside the right region, the result is garbage



Cat images: Joaquim Alves Gaspar CC-SA

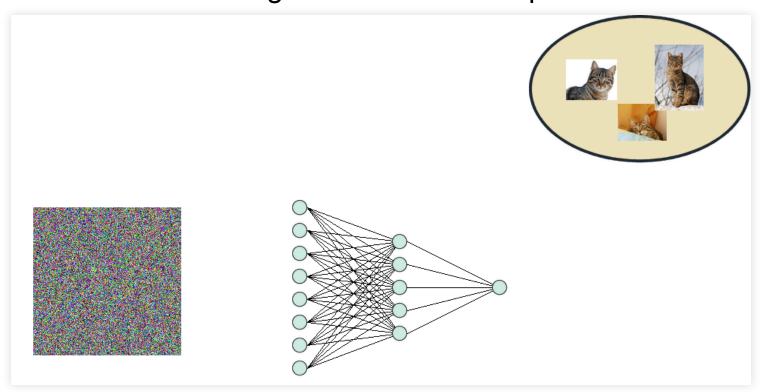
#### Generative adversarial networks

- Fix the latent space with some distribution
- The result will be garbage because net not trained



#### **Generative adversarial networks**

Train a network to distinguish the real examples from fakes



#### **Generative adversarial networks**

- One network creates examples from given distribution
- The other distinguishes real from fake
- Train both, alternating, so each becomes increasingly better



Ian Goodfellow

# **Generating Data**

#### Generative adversarial networks

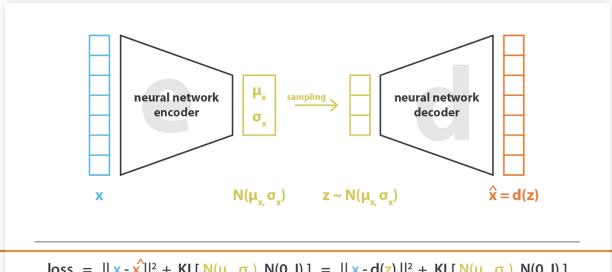
- One network creates examples from given distribution
- The other distinguishes real from fake
- Train both, alternating, so each becomes increasingly better
- As a result, the generator learns to map our fixed initial distribution to the space of our target examples.

# **Generating Data**

- Can we use autoencoders to generate new examples?
- Yes, if we know the "shape" of the latent space

#### Variational Autoencoders

- Train the autoencoder to encode into a given distribution
- E.g. mixture of independent Gaussians
- This way we learn the distribution for generating examples of each type



#### Variational Autoencoders

- How do we backpropagate through random sampling?
- Reparametrize: z is deterministic apart from a normally distributed error

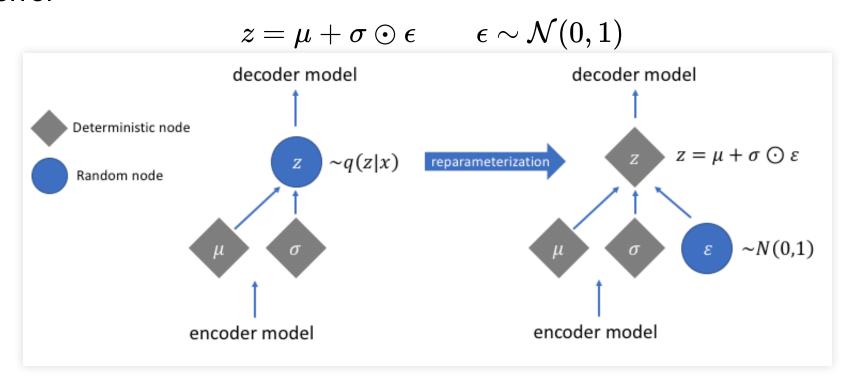
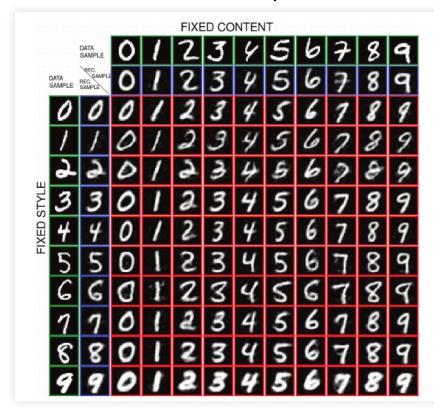


Image: Jeremy Jordan, Variational autoencoders.

### Variational Autoencoders

- VAE can learn to disentangle meaningful attributes
- We can force the independence of the latent variables



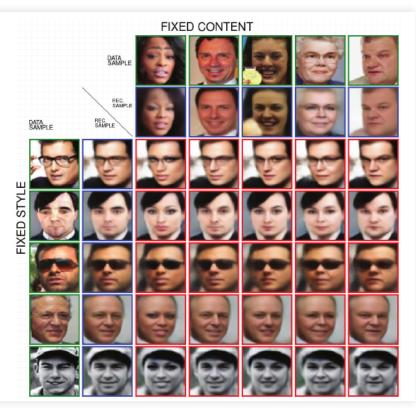


Image: Bouchacourt et. al., Multi-level variational autoencoder, 2018

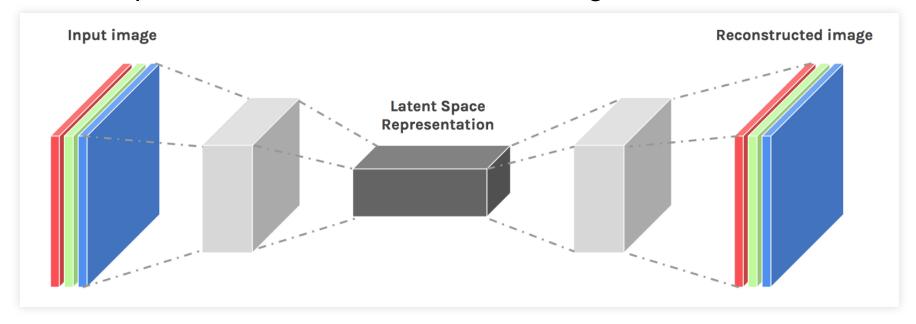
## Autoencoders

# **Convolutional Autoencoders**

### Convolutional Autoencoders

## Use convolutions and upsampling to reconstruct

Latent space is narrow, need to restore original dimensions

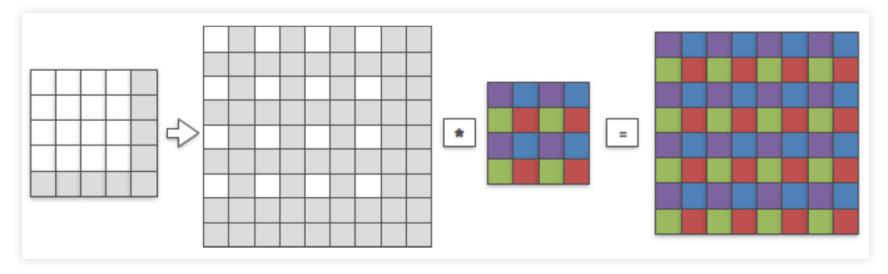


Barna Pásztor, Aligning hand-written digits with Convolutional Autoencoders

#### Convolutional Autoencoders

Upsample followed by convolution (in 2D)

```
from tensorflow.keras.layers import UpSampling1D,UpSampling2D
UpSampling1D(size=2)
UpSampling2D(size=(2, 2), data_format=None, interpolation='nearest')
```

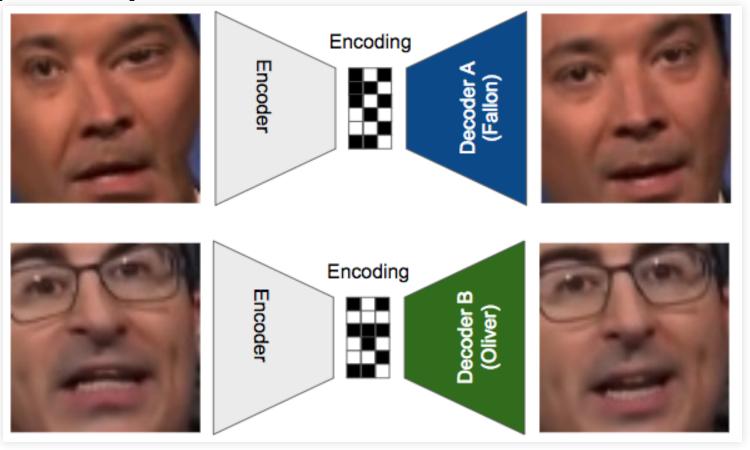


Shi et. al., Is the deconvolution layer the same as a convolutional layer?

## **Example: deep fakes**

- Train the same encoder on different sets of inputs
- But for each set reconstruct with a specific decoder
- With this we can "translate" between sets

# **Example: deep fakes**



Gaurav Oberoi, Exploring DeepFakes, https://goberoi.com/exploring-deepfakes-20c9947c22d9

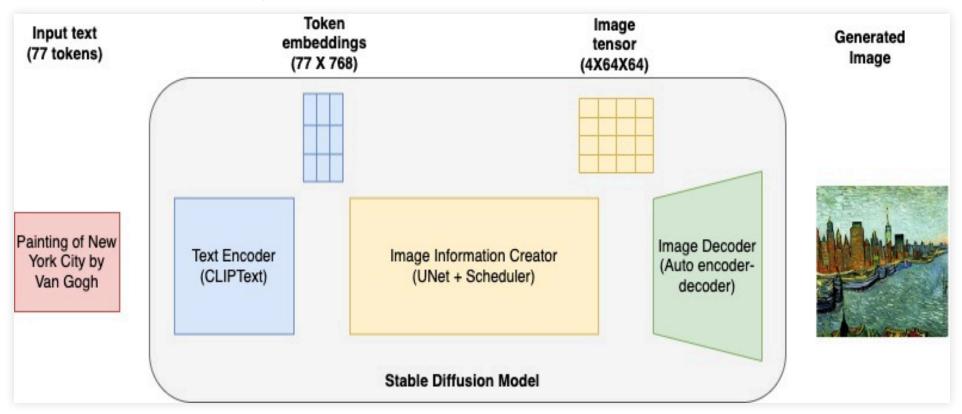
## **Example:** deep fakes

- Train with images from videos
- Process video:
- Input Fallon to encoder
- Output Oliver using Oliver decoder



#### **Example: Text-to-image**

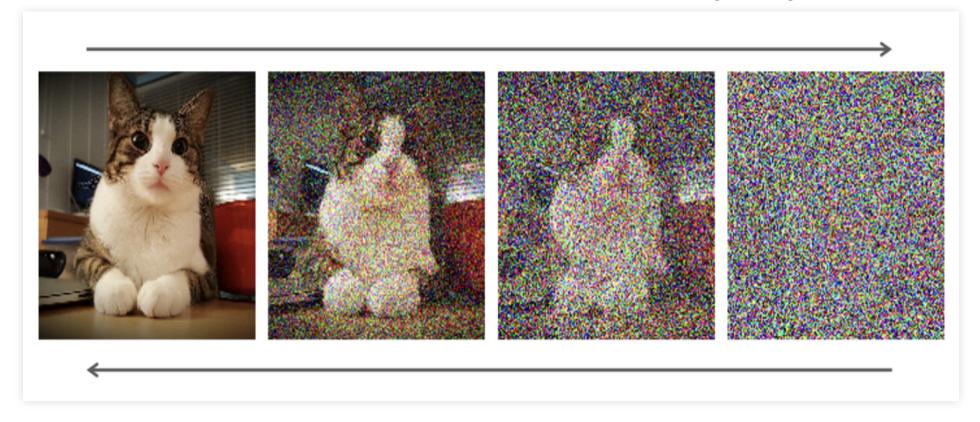
Stable Diffusion, DALL-e



Amazon Machine Learning Blog, https://aws.amazon.com/blogs/machine-learning/create-high-quality-images-with-stable-diffusion-models-and-deploy-them-cost-efficiently-with-amazon-sagemaker/

## **Example: Text-to-image**

Based on U-Net model architecture: CNN for image segmentation



Edge AI and vision, https://www.edge-ai-vision.com/2023/01/from-dall%C2%B7e-to-stable-diffusion-how-do-text-to-image-generation-models-work/

# Autoencoders

# Summary

#### Autoencoders

#### **Summary**

- Autoencoders: learn the input in the output
- Unsupervised learning
- Using restrictions (dimension, regularization)
- Or reconstruction (from corrupted inputs)
- Convolutional Autoencoders
- Recent applications

#### **Further reading:**

Goodfellow et.al, Deep learning, Chapter 14