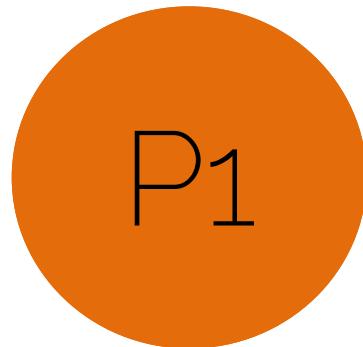


Lecture 11 Recap

Transfer Learning

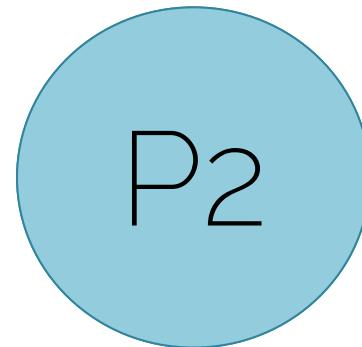
Distribution



Large dataset



Distribution



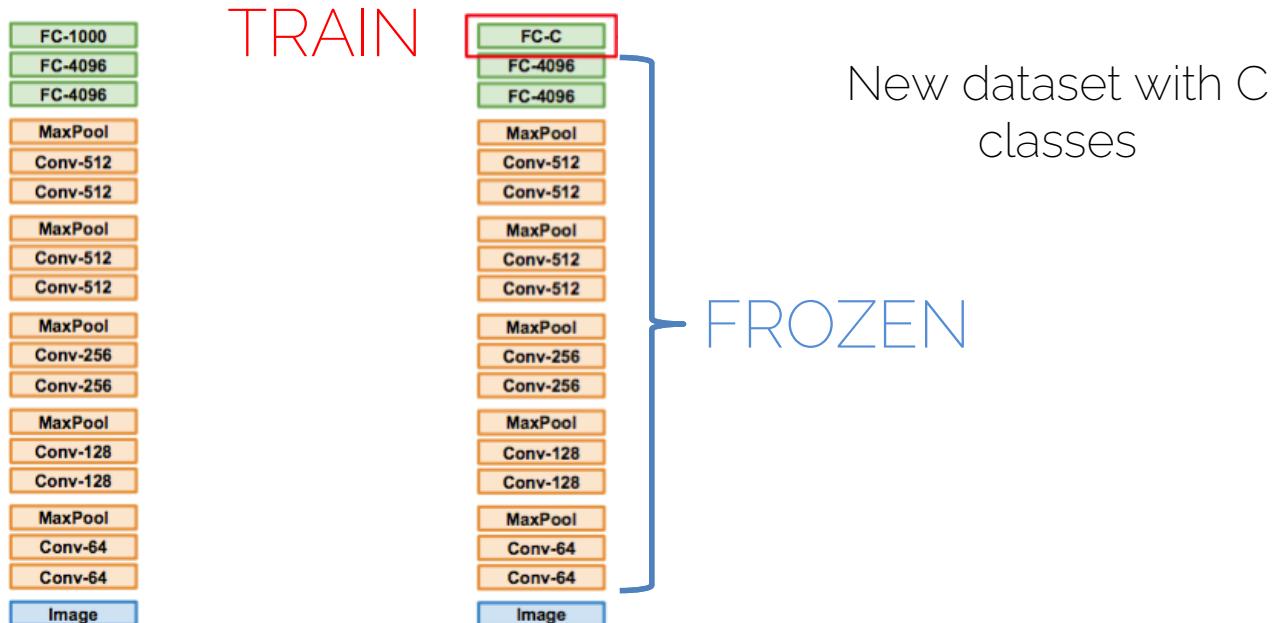
Small dataset



Use what has been
learned for another
setting

Transfer Learning

Trained on ImageNet

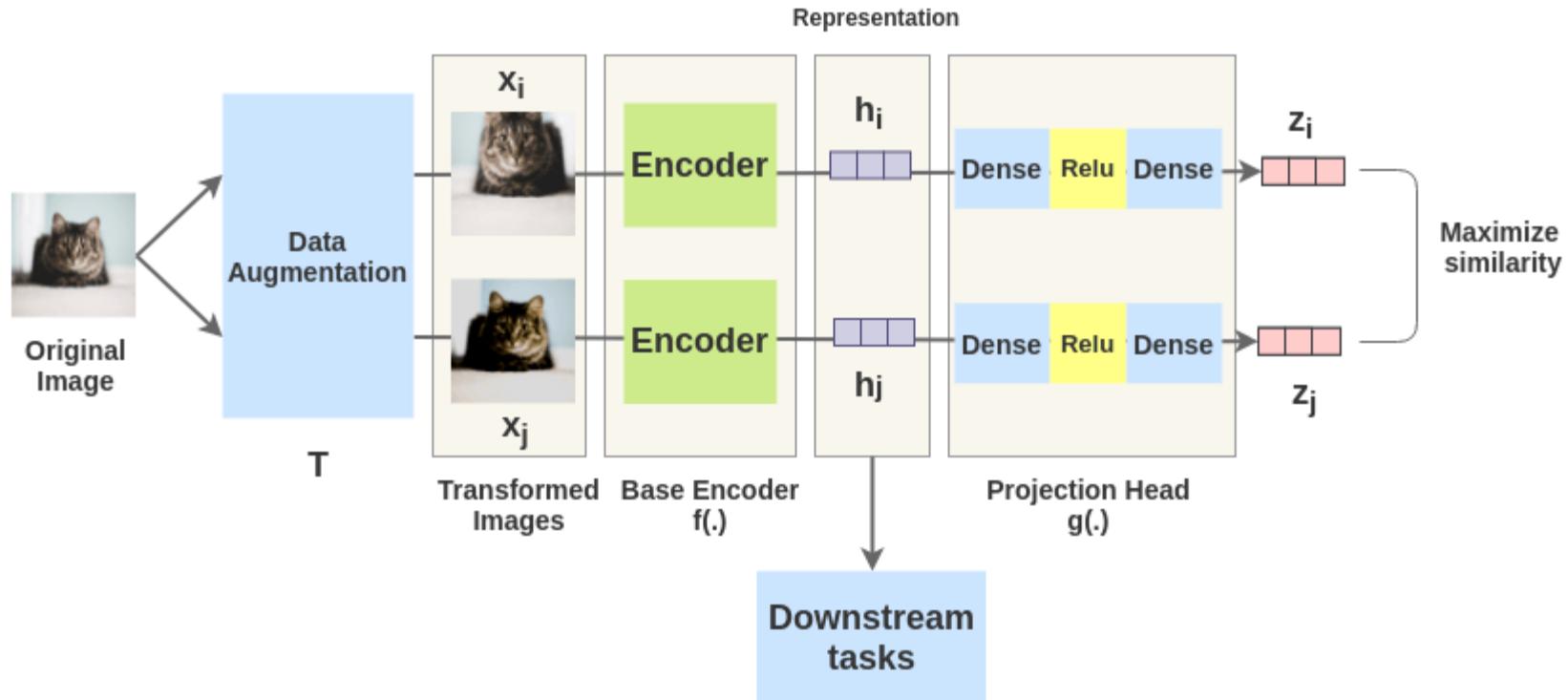


Source : http://cs231n.stanford.edu/slides/2016/winter1516_lecture11.pdf

[Donahue et al., ICML'14] DeCAF,

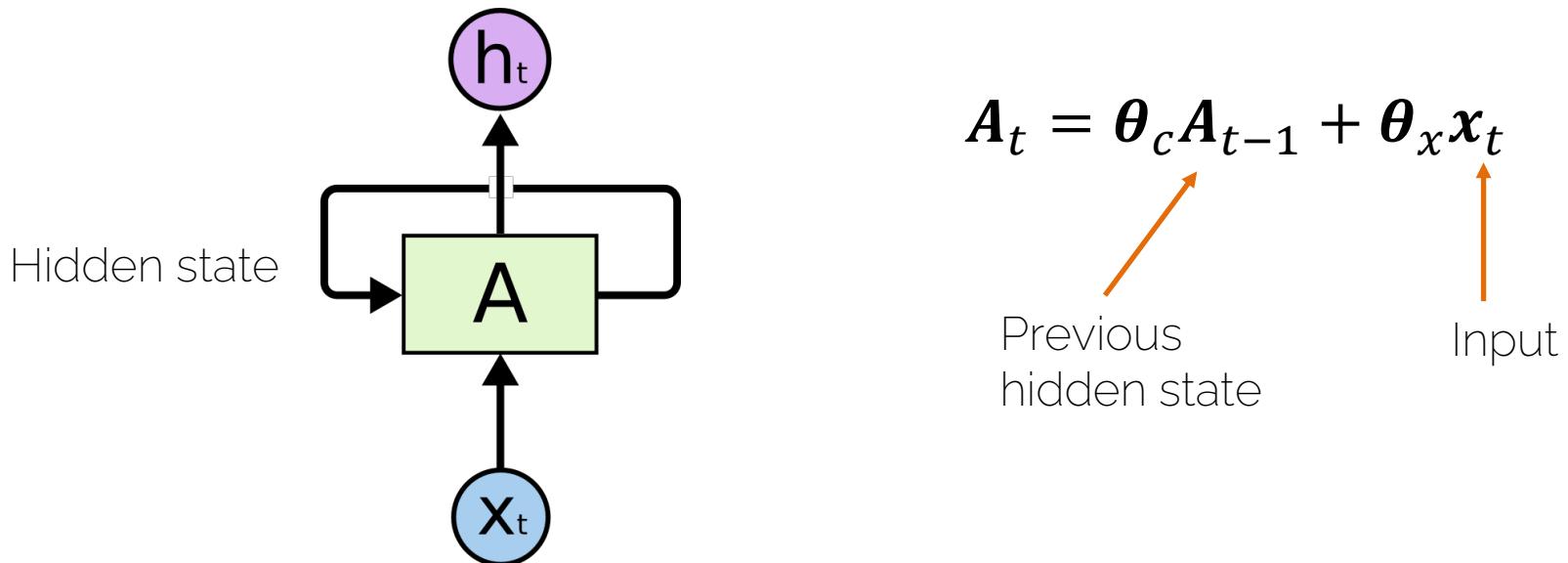
[Razavian et al., CVPRW'14] CNN Features off-the-shelf

Representation Learning



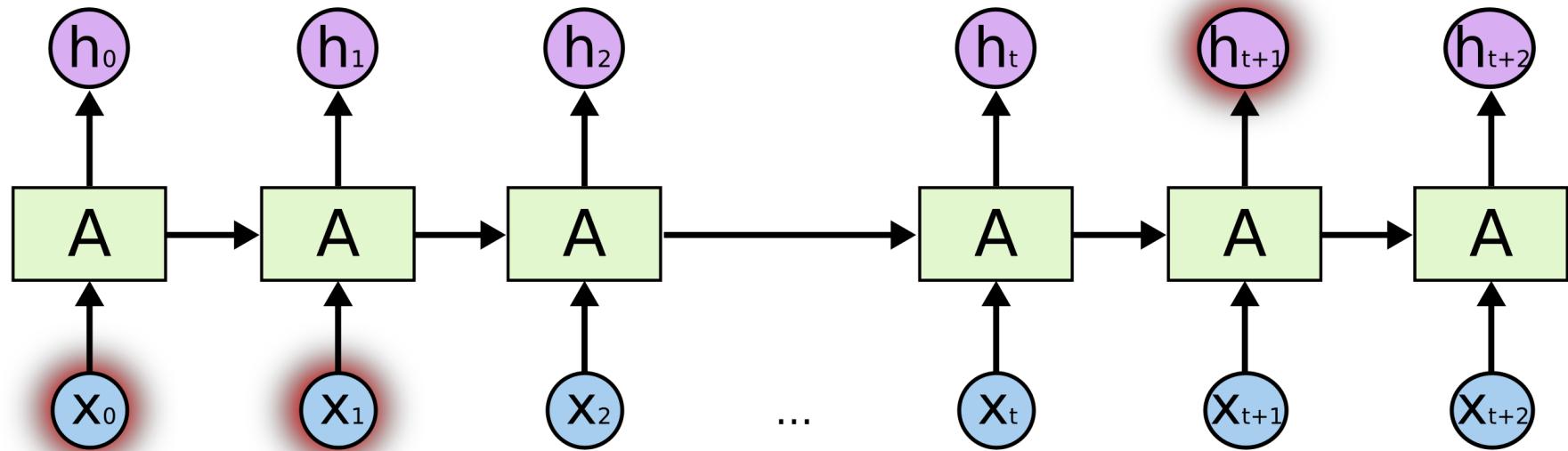
Basic Structure of RNN

- We want to have notion of "time" or "sequence"



Source: <https://colah.github.io/posts/2015-08-Understanding-LSTMs/>

Long-Term Dependencies

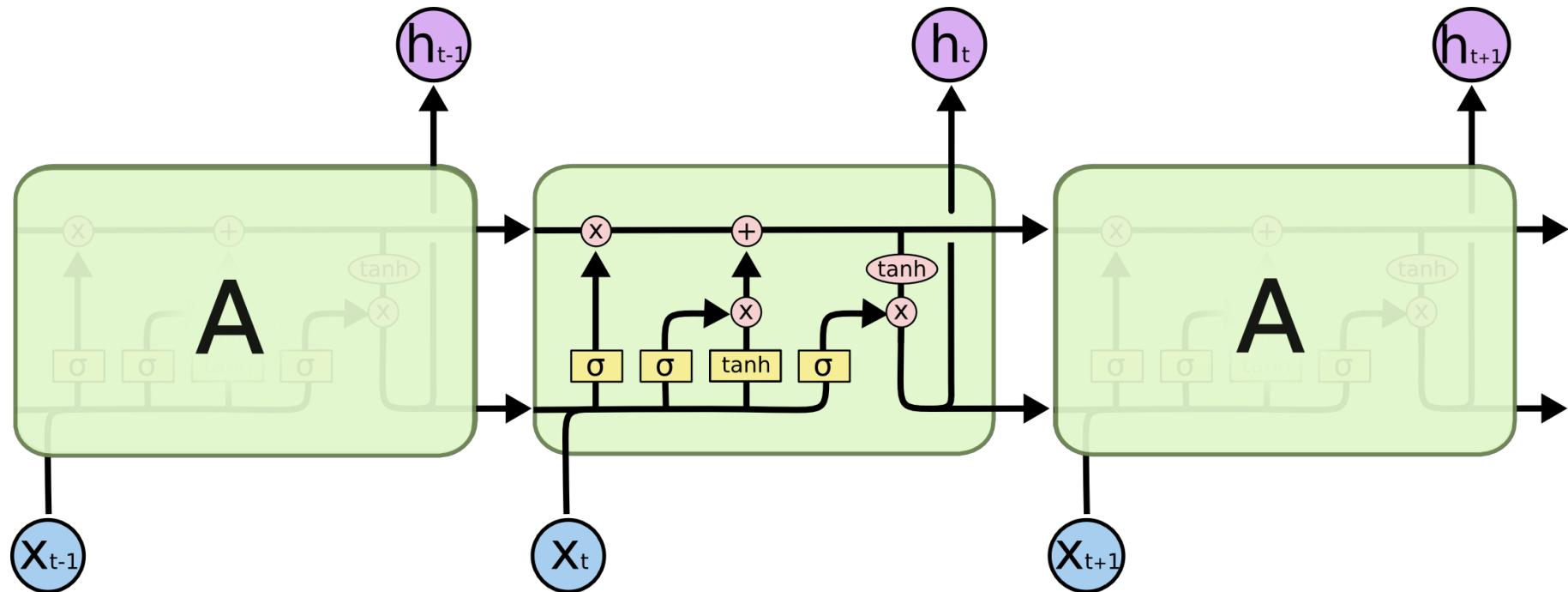


I moved to Germany ...

so I speak German fluently.

Source: <https://colah.github.io/posts/2015-08-Understanding-LSTMs/>

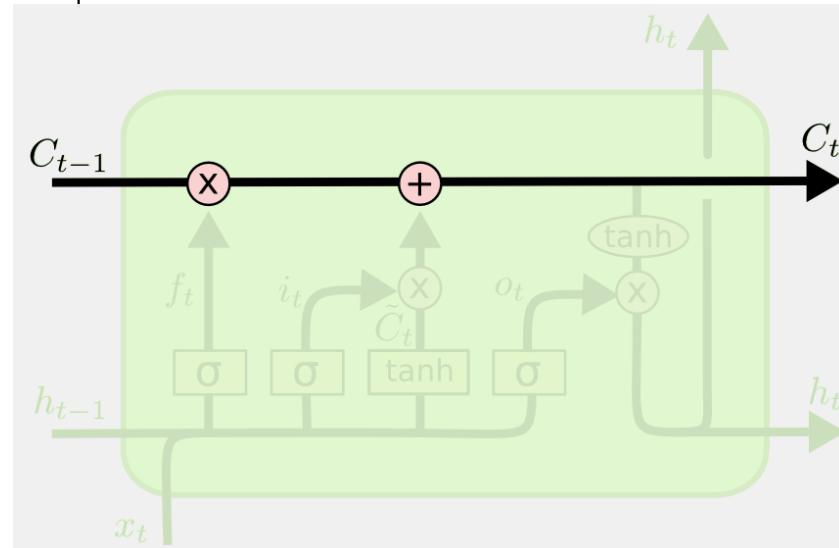
Long-Short Term Memory Units(LSTM)



Source: <https://colah.github.io/posts/2015-08-Understanding-LSTMs/>

Long-Short Term Memory Units

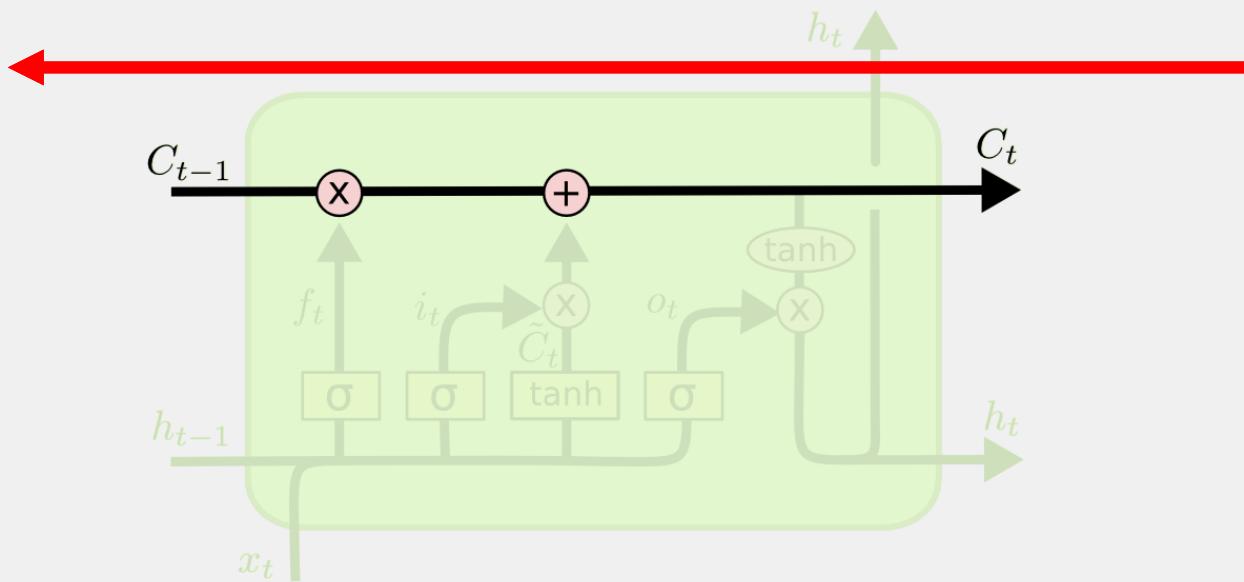
- Key ingredients
- Cell = transports the information through the unit



Source: <https://colah.github.io/posts/2015-08-Understanding-LSTMs/>

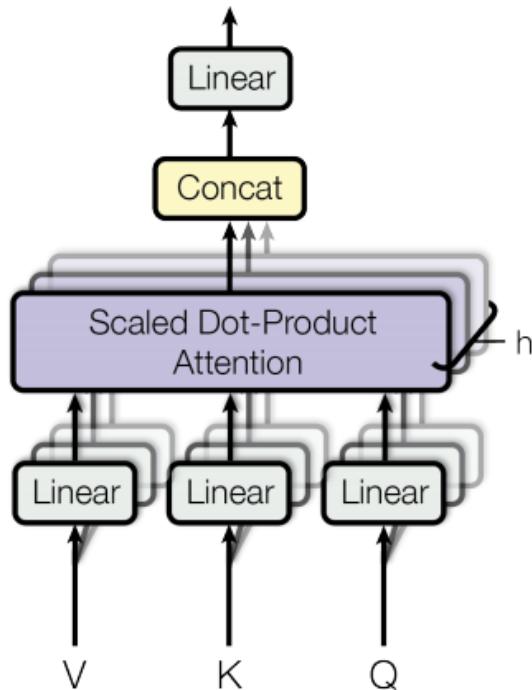
LSTM

- Highway for the gradient to flow



Source: <https://colah.github.io/posts/2015-08-Understanding-LSTMs/>

Attention



Intuition: Take the query Q , find the most similar key K , and then find the value V that corresponds to the key.

In other words, learn V , K , Q where:

- V – here is a bunch of interesting things.
- K – here is how we can index some things.
- Q – I would like to know this interesting thing.

Loosely connected to Neural Turing Machines (Graves et al.).

Attention

Index the values via a differentiable operator.

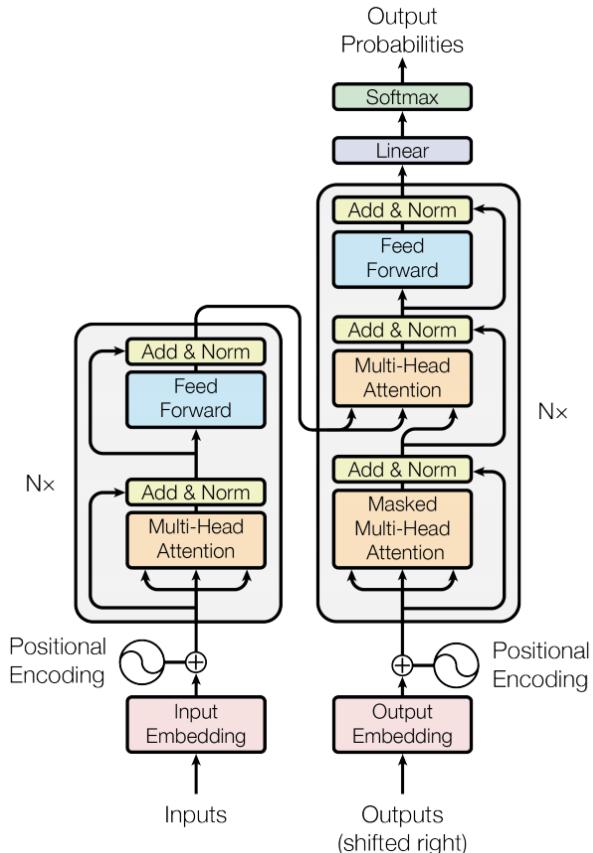
Multiply queries with keys

Get the values

$$\text{Attention}(Q, K, V) = \text{softmax} \left(\frac{QK^T}{\sqrt{d_k}} \right) V$$

To train them well, divide by $\sqrt{d_k}$, "probably" because for large values of the key's dimension, the dot product grows large in magnitude, pushing the softmax function into regions where it has extremely small gradients.

Transformers

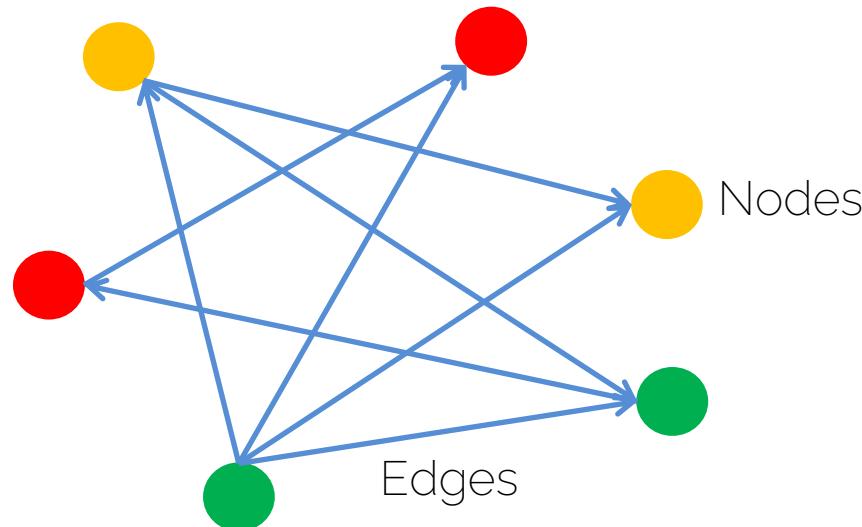


Lecture 12: Advanced DL topics

Graph Neural Networks

A graph

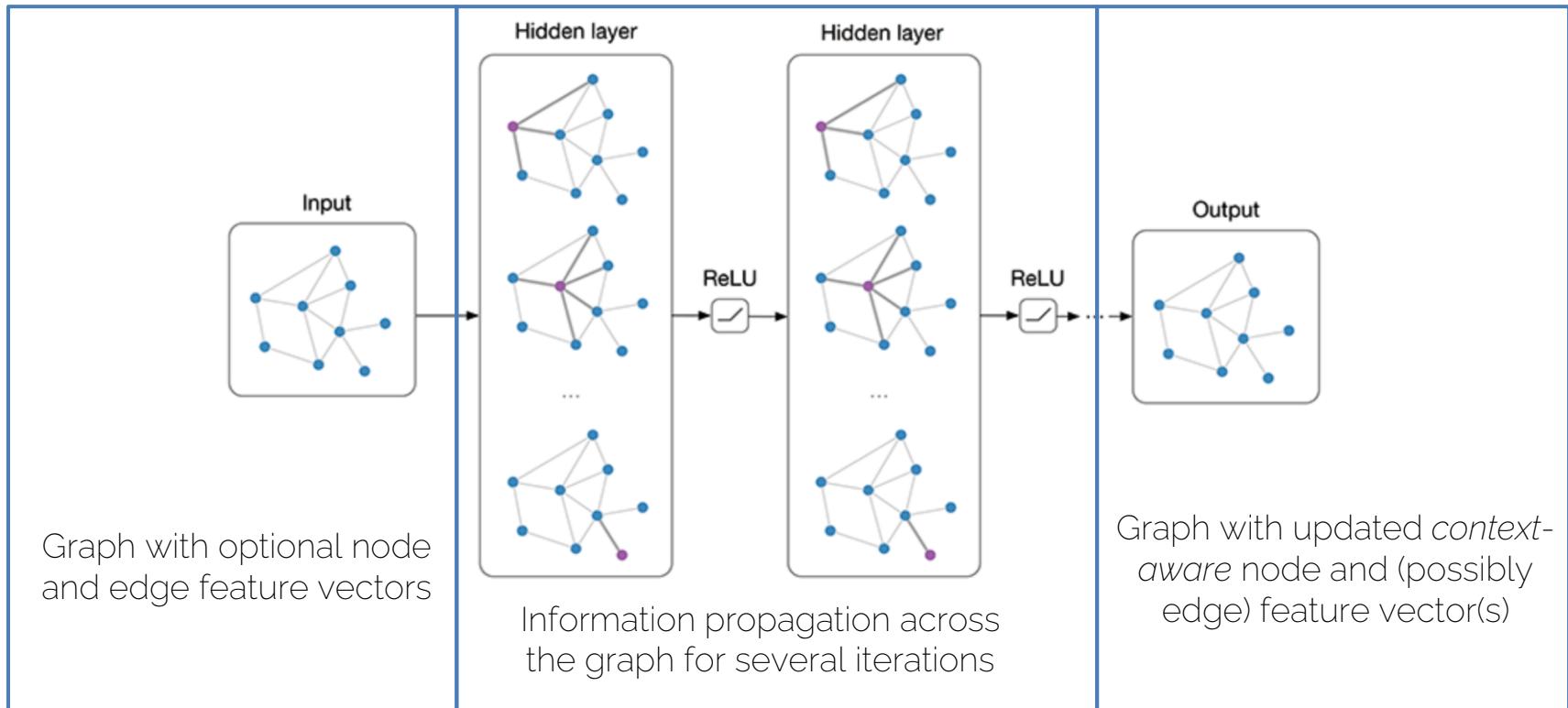
- Node: a concept
- Edge: a connection between concepts



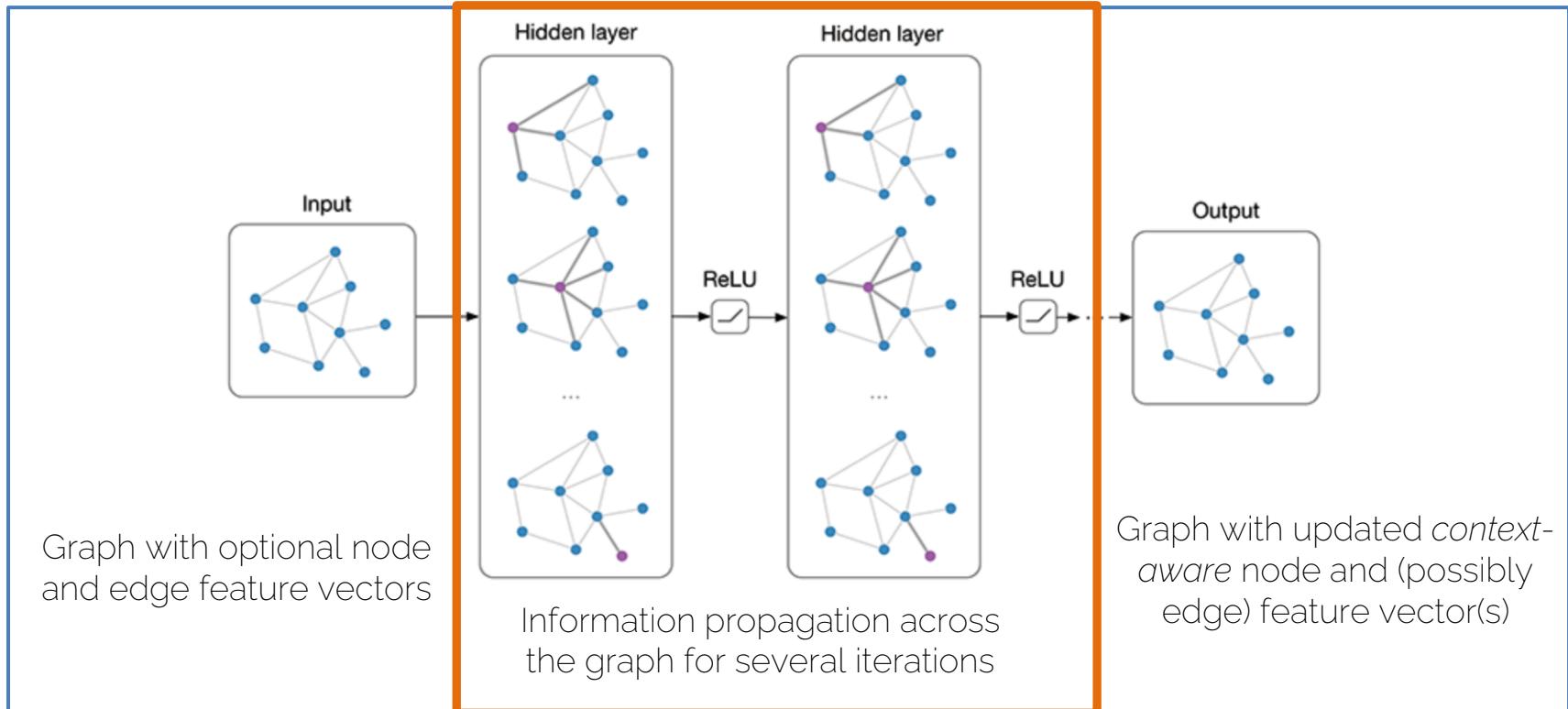
Deep learning on graphs

- Generalizations of neural networks that can operate on graph-structured domains:
 - Scarselli et al. "The Graph Neural Network Model". IEEE Trans. Neur. Net 2009.
 - Kipf et al. "Semi-Supervised Classification with Graph Convolutional Networks. ICLR 2016.
 - Gilmer et al. "Neural Message Passing for Quantum Chemistry". ICML 2017
 - Battaglia et al. "Relational inductive biases, deep learning, and graph networks". arXiv 2018 (review paper)
- Key challenges:
 - Variable sized inputs (number of nodes and edges)
 - Need invariance to node permutations

General Idea

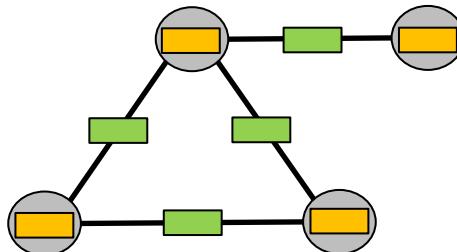


General Idea

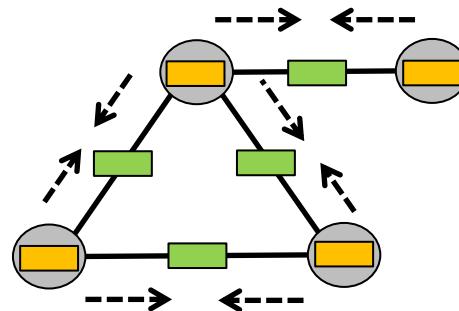


Message Passing Networks

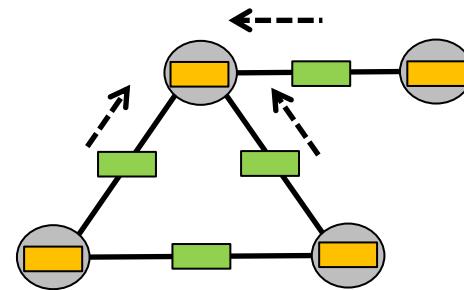
- We can divide the propagation process in two steps: 'node to edge' and 'edge to node' updates.



Initial Graph



'Node to Edge' Update



'Edge to Node' Update

Node embeddings
 Edge embeddings

'Node to edge' updates

- At every message passing step l , first do:

$$h_{(i,j)}^{(l)} = \mathcal{N}_e \left([h_i^{(l-1)}, h_{(i,j)}^{(l-1)}, h_j^{(l-1)}] \right)$$

The diagram illustrates the inputs to the function \mathcal{N}_e . Three orange arrows point from the text descriptions below to the corresponding terms in the equation: the left arrow points to $h_i^{(l-1)}$, the middle arrow points to $h_{(i,j)}^{(l-1)}$, and the right arrow points to $h_j^{(l-1)}$.

Embedding of node i in the previous message passing step

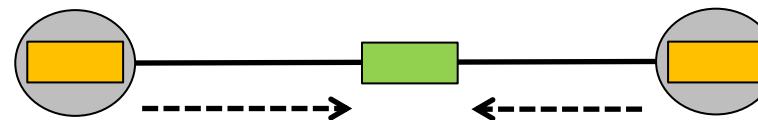
Embedding of edge (i,j) in the previous message passing step

Embedding of node j in the previous message passing step

'Node to edge' updates

- At every message passing step l , first do:

$$h_{(i,j)}^{(l)} = \mathcal{N}_e \left([h_i^{(l-1)}, h_{(i,j)}^{(l-1)}, h_j^{(l-1)}] \right)$$

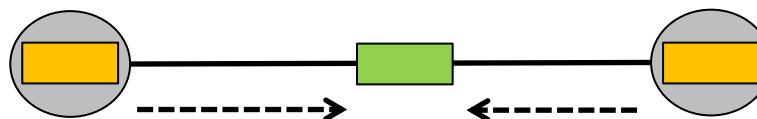


'Node to edge' updates

- At every message passing step l , first do:

$$h_{(i,j)}^{(l)} = \underbrace{\mathcal{N}_e}_{\text{Learnable function}} \left([h_i^{(l-1)}, h_{(i,j)}^{(l-1)}, h_j^{(l-1)}] \right)$$

Learnable function (e.g.
MLP) with shared
weights across the
entire graph



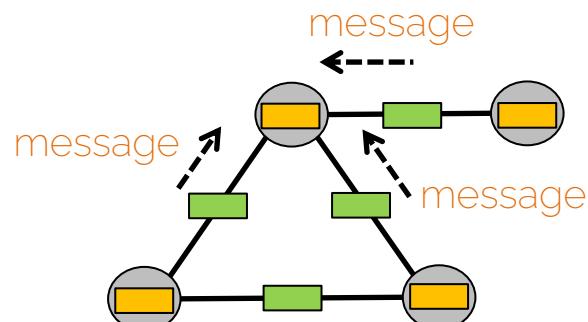
'Edge to node' updates

- After a round of edge updates, each edge embedding contains information about its pair of incident nodes
- Then, edge embeddings are used to update nodes:

$$m_i^{(l)} = \Phi \left(\left\{ h_{(i,j)}^{(l)} \right\}_{j \in N_i} \right)$$

Order invariant
operation (e.g.
sum, mean, max)

Neighbors of
node i



'Edge to node' updates

- After a round of edge updates, each edge embedding contains information about its pair of incident nodes
- Then, edge embeddings are used to update nodes:

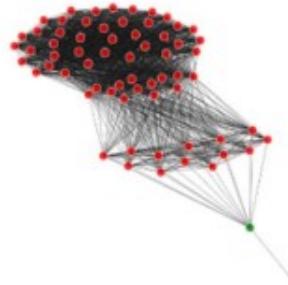
$$m_i^{(l)} = \Phi \left(\left\{ h_{(i,j)}^{(l)} \right\}_{j \in N_i} \right)$$
$$h_i^{(l)} = \mathcal{N}_v \left([m_i^{(l)}, h_i^{(l-1)}] \right)$$

The aggregation provides each node embedding with contextual information about its neighbors

Learnable function (e.g. MLP) with shared weights across the entire graph

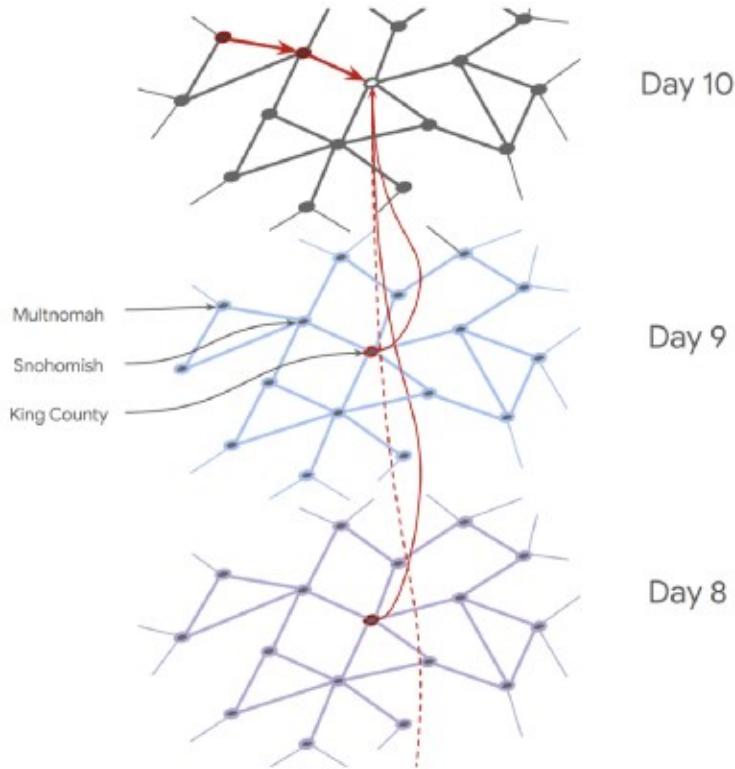
GNN Applications

- Node or edge classification
 - identifying anomalies such as spam, fraud
 - Relationship discovery for social networks, search networks



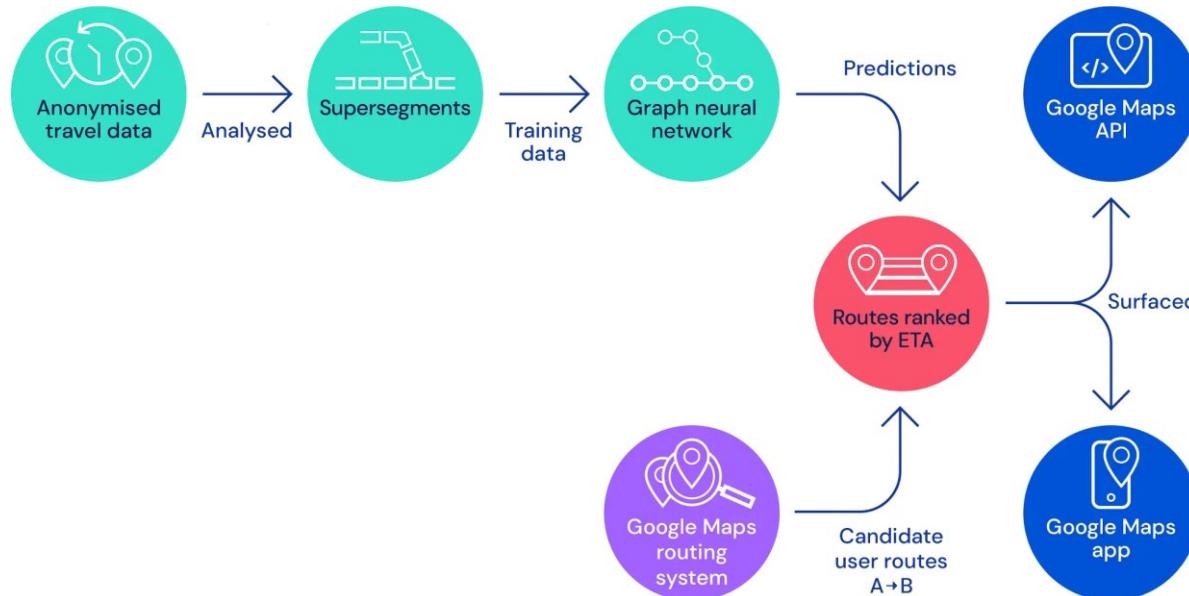
GNN Applications

- Modeling epidemiology
 - Spatio-temporal graph



GNN Applications

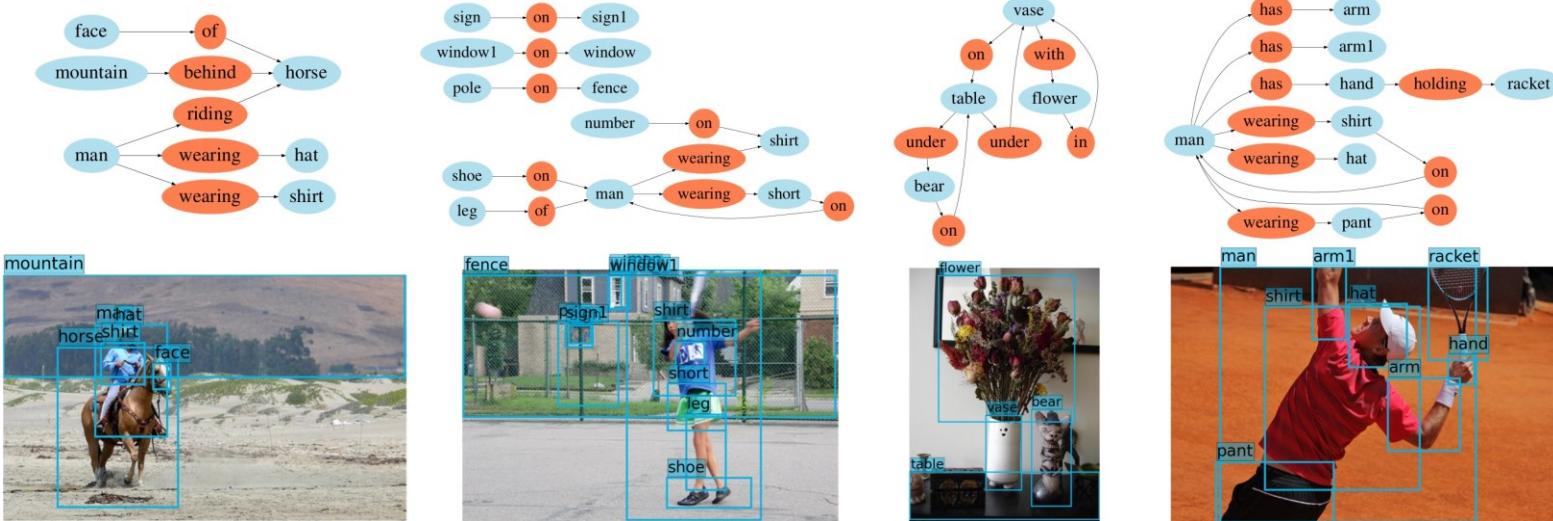
- Traffic forecasting



<https://www.deepmind.com/blog/traffic-prediction-with-advanced-graph-neural-networks>

GNN Applications

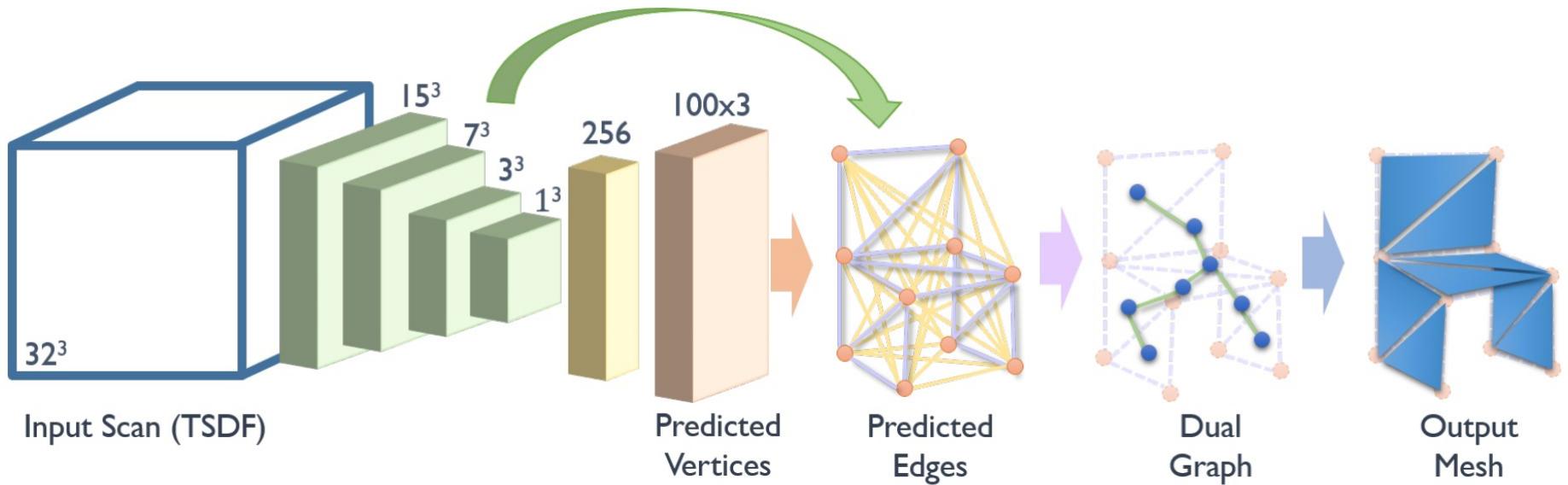
- Scene graph generation



[Xu et al. '17] Scene Graph Generation by Iterative Message Passing

GNN Applications

- 3D mesh generation

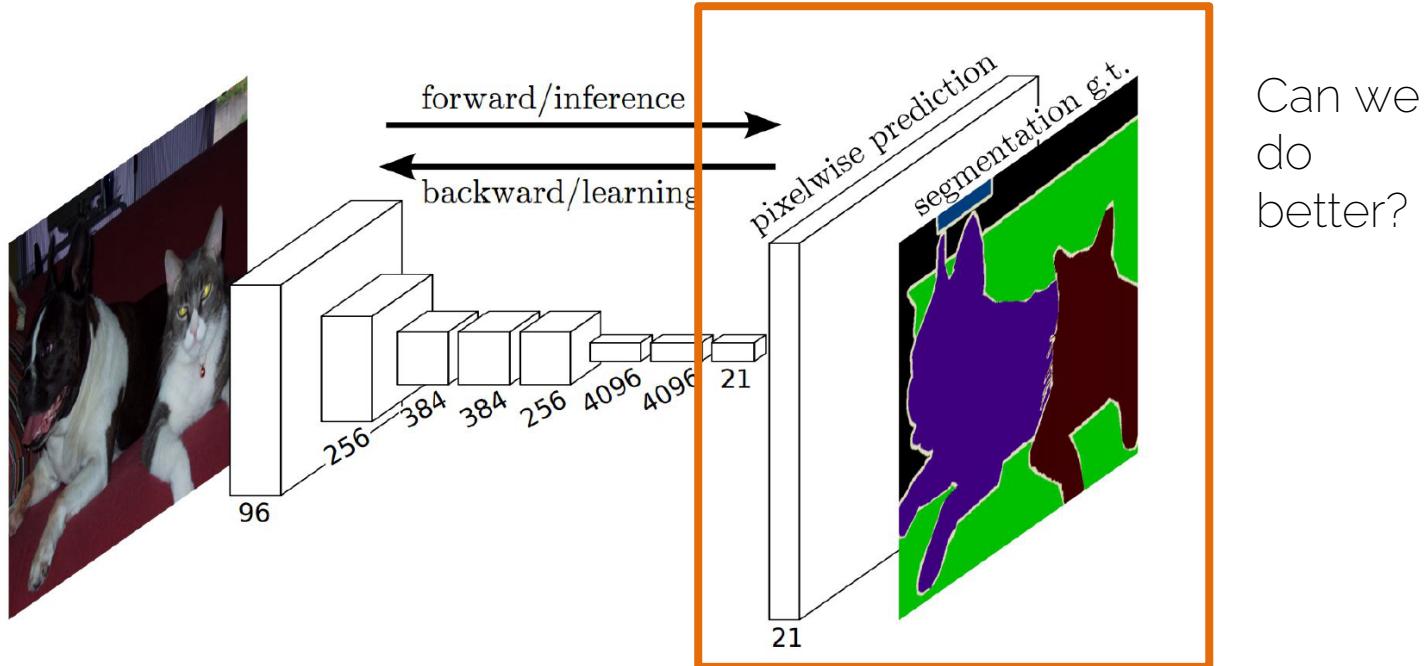


[Dai and Niessner] Scan2Mesh: From Unstructured Range Scans to 3D Meshes

Generative Models

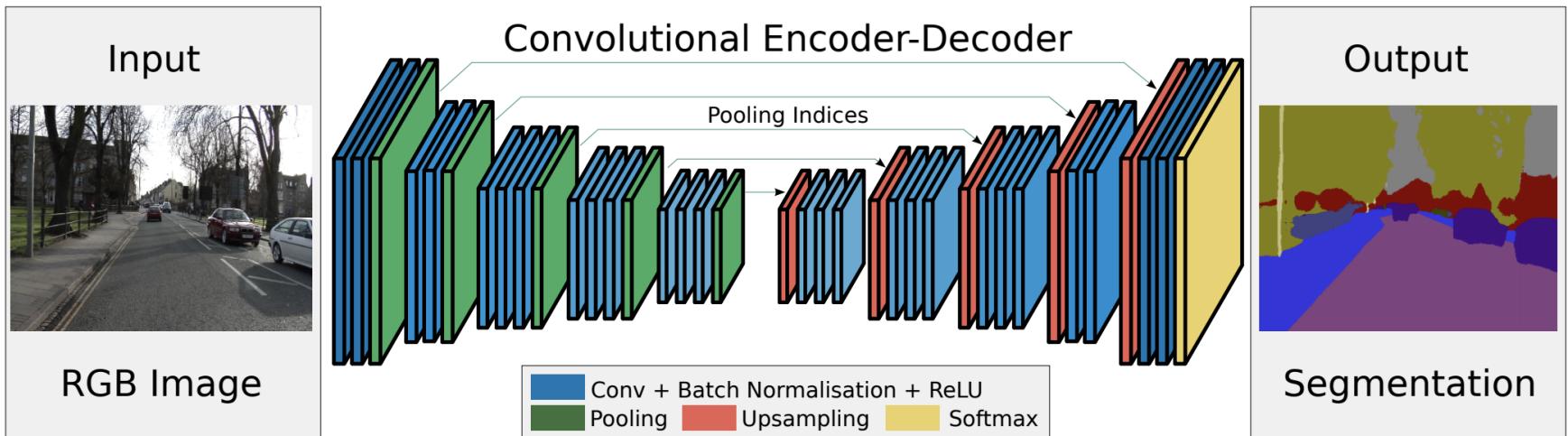
Semantic Segmentation (FCN)

- Recall the Fully Convolutional Networks



[Long et al., CVPR'15] : Fully Convolutional Networks for Semantic Segmentation

SegNet

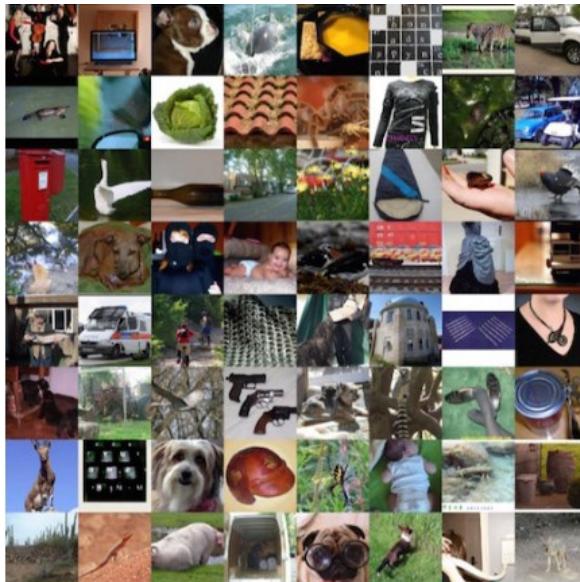


[Badrinarayanan et al., TPAMI'16] SegNet: A Deep Convolutional Encoder-Decoder Architecture for Image Segmentation
I2DL: Prof. Dai

Generative Models

- Given training data, how to generate new samples from the same distribution

Real Images



Generated Images



Generative Models

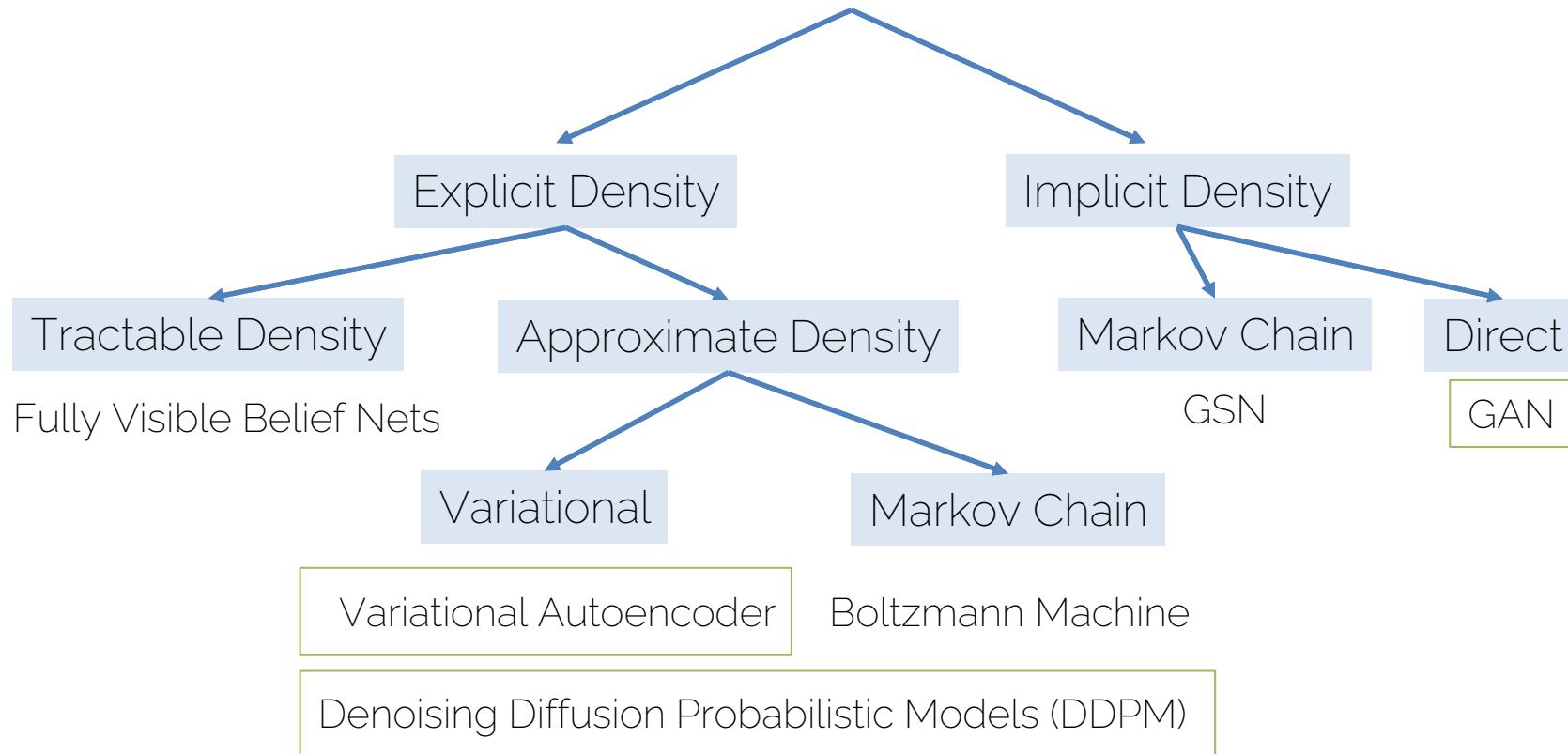
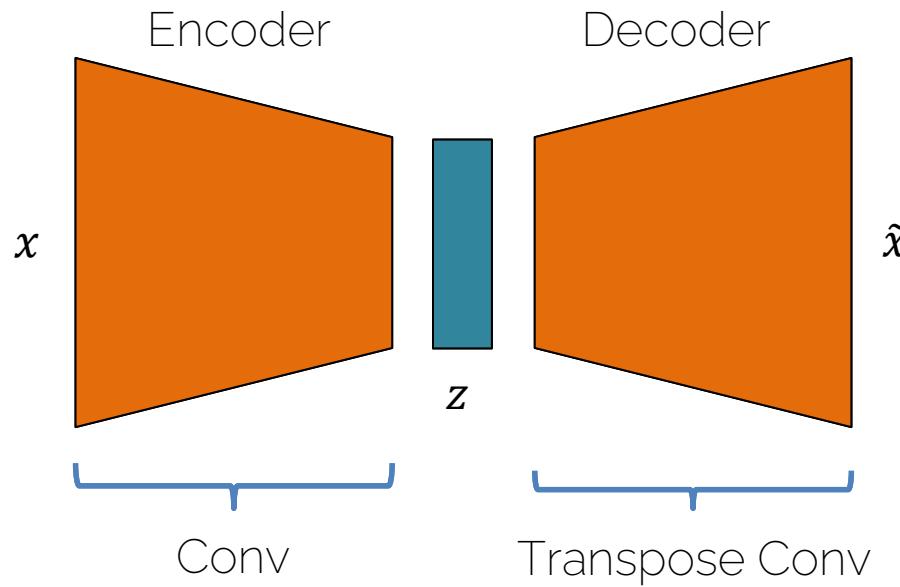


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017

Variational Autoencoders

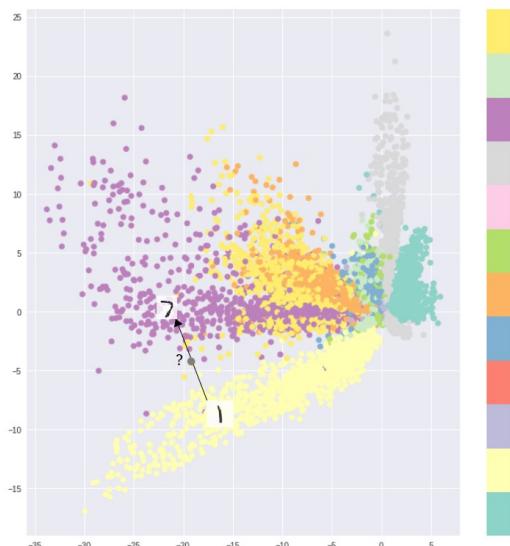
Autoencoders

- Encode the input into a representation (bottleneck) and reconstruct it with the decoder



Autoencoders

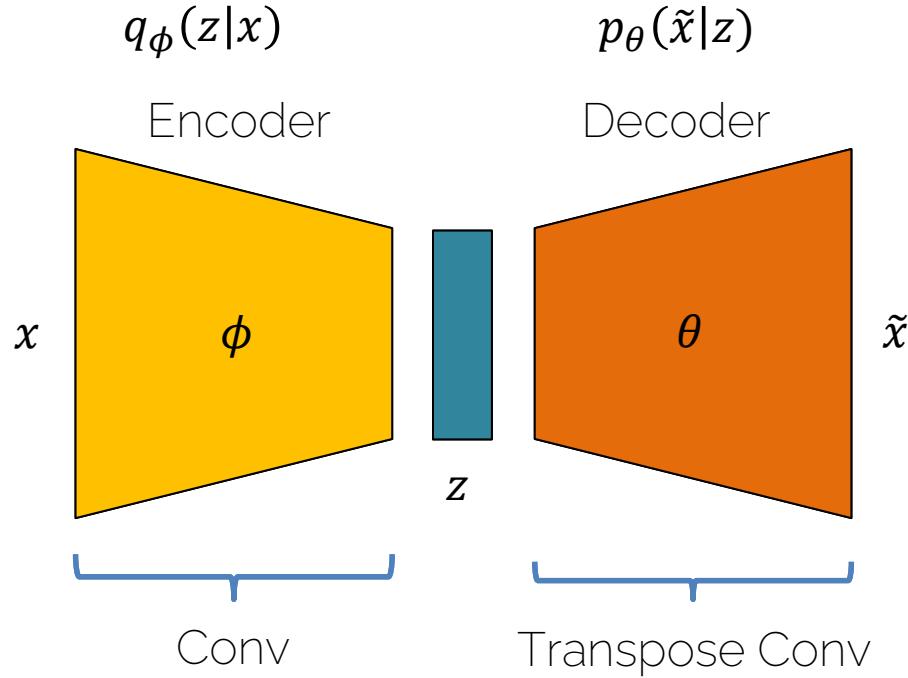
- Encode the input into a representation (bottleneck) and reconstruct it with the decoder



Latent space learned
by autoencoder on MNIST

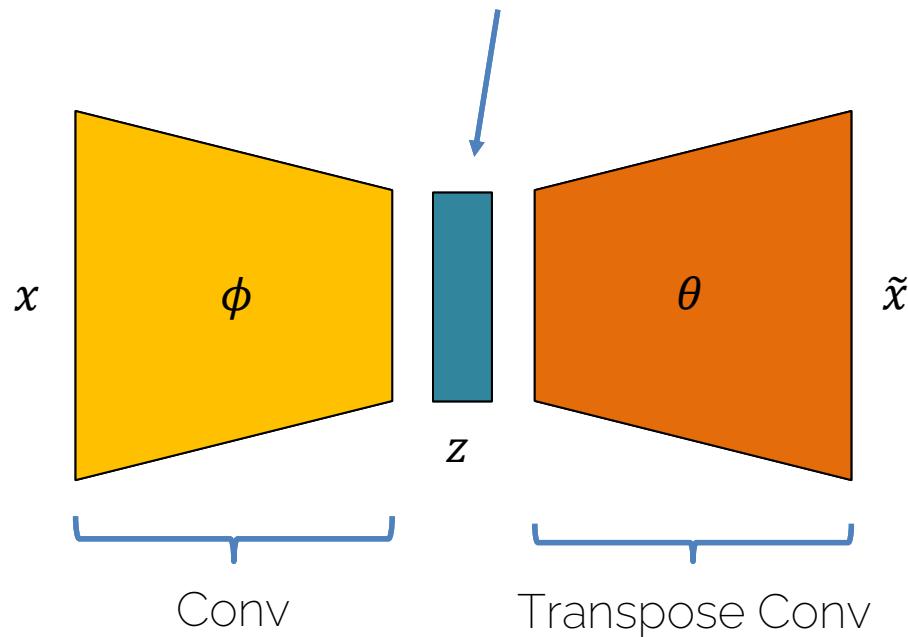
Source: <https://bit.ly/37ctFMS>

Variational Autoencoder



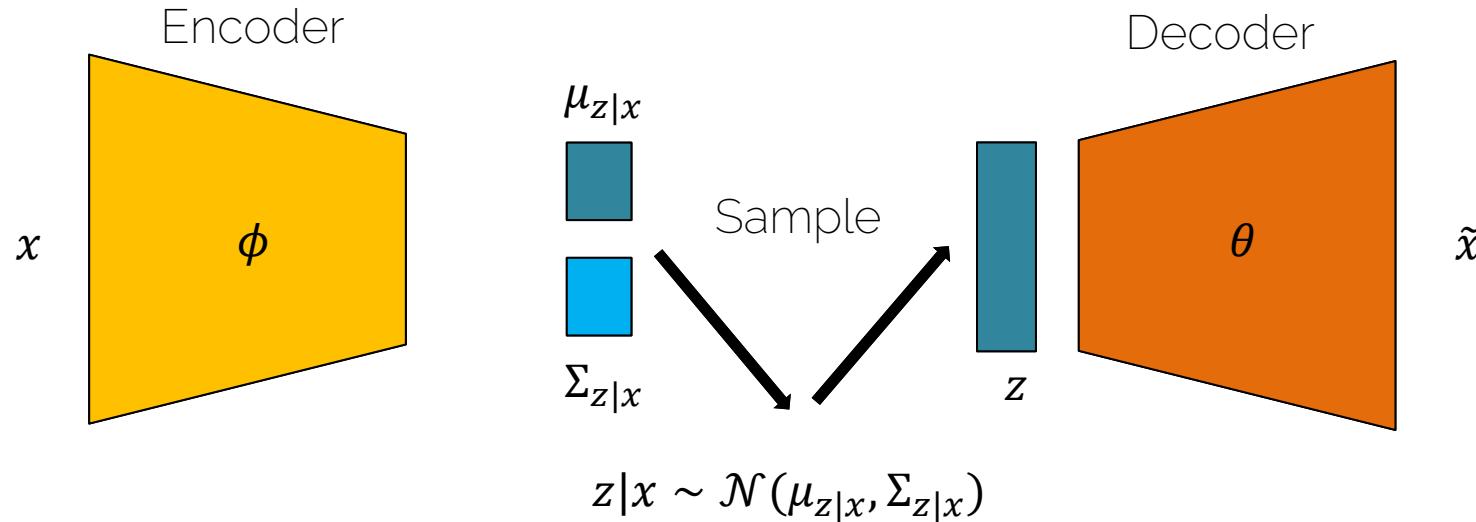
Variational Autoencoder

Goal: Sample from the latent distribution to generate new outputs!



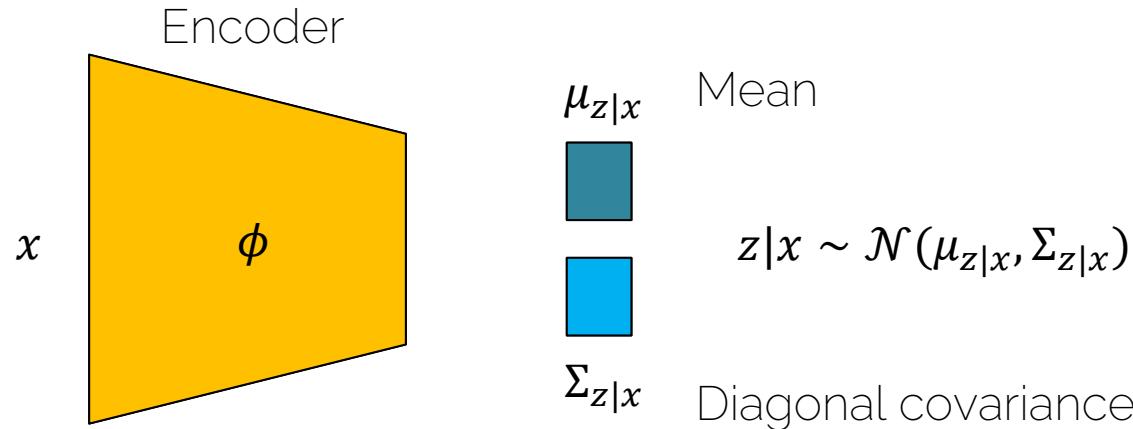
Variational Autoencoder

- Latent space is now a distribution
- Specifically it is a Gaussian



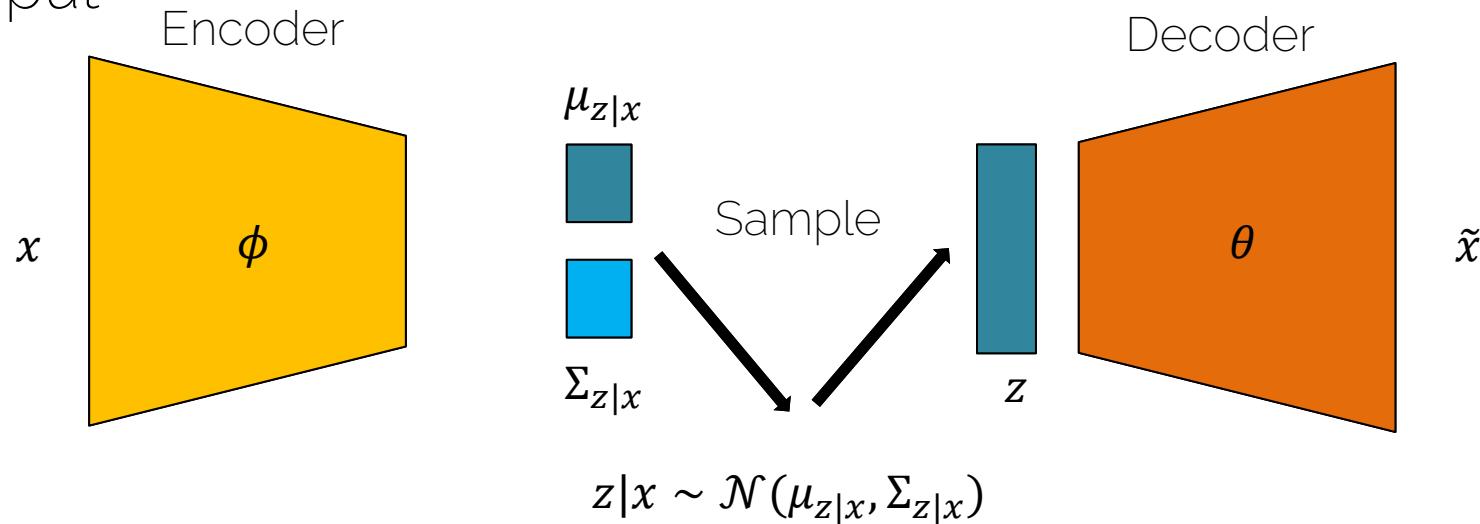
Variational Autoencoder

- Latent space is now a distribution
- Specifically it is a Gaussian



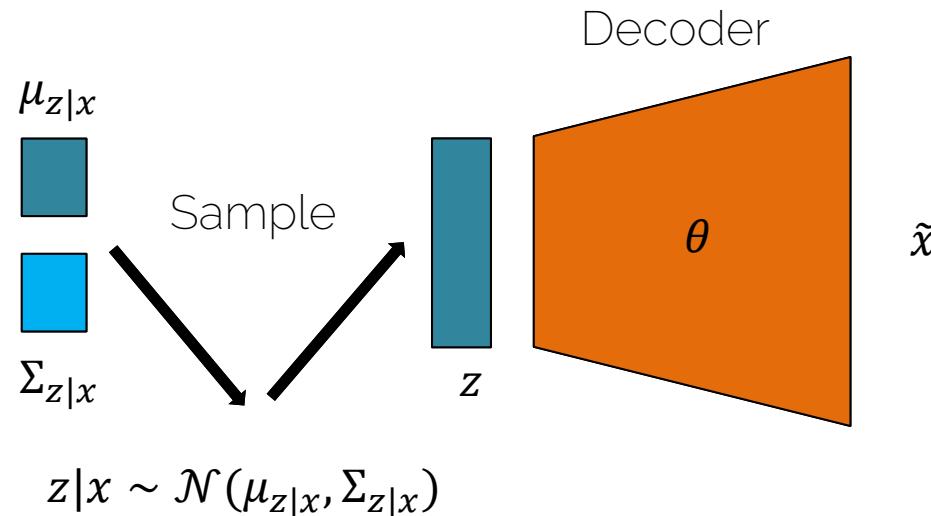
Variational Autoencoder

- Training: loss makes sure the latent space is close to a Gaussian and the reconstructed output is close to the input



Variational Autoencoder

- Test: Sample from the latent space



Autoencoder vs VAE



Autoencoder



Variational Autoencoder



Ground Truth

Source: <https://github.com/kvfrans/variational-autoencoder>

Generating data

Degree of smile



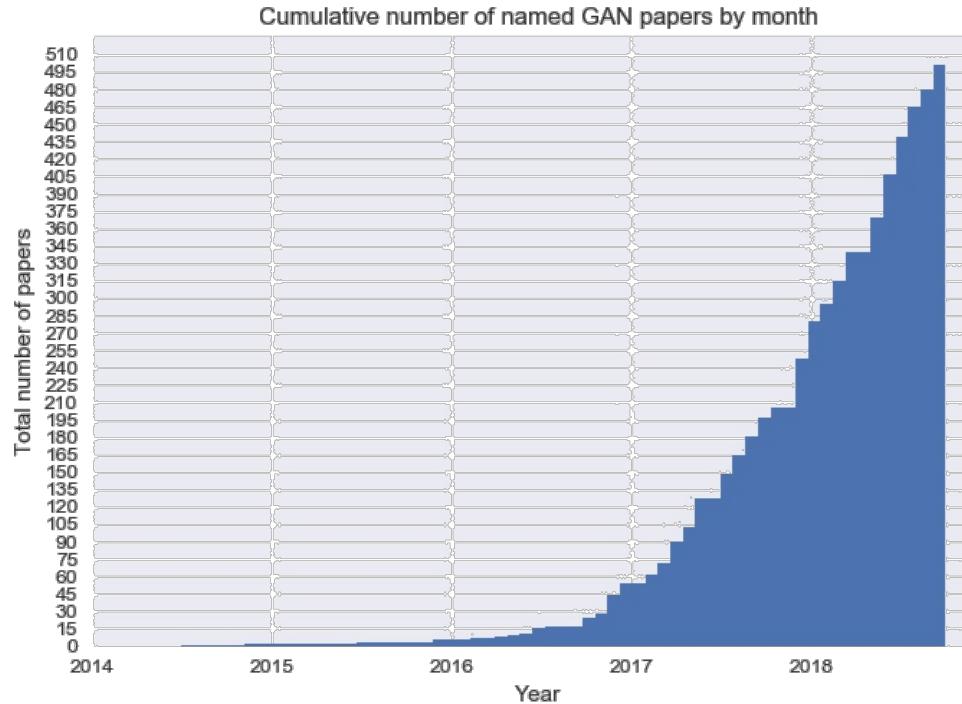
Head pose

Autoencoder Overview

- Autoencoders (AE)
 - Reconstruct input
 - Unsupervised learning
- Variational Autoencoders (VAE)
 - Probability distribution in latent space (e.g., Gaussian)
 - Interpretable latent space (head pose, smile)
 - Sample from model to generate output

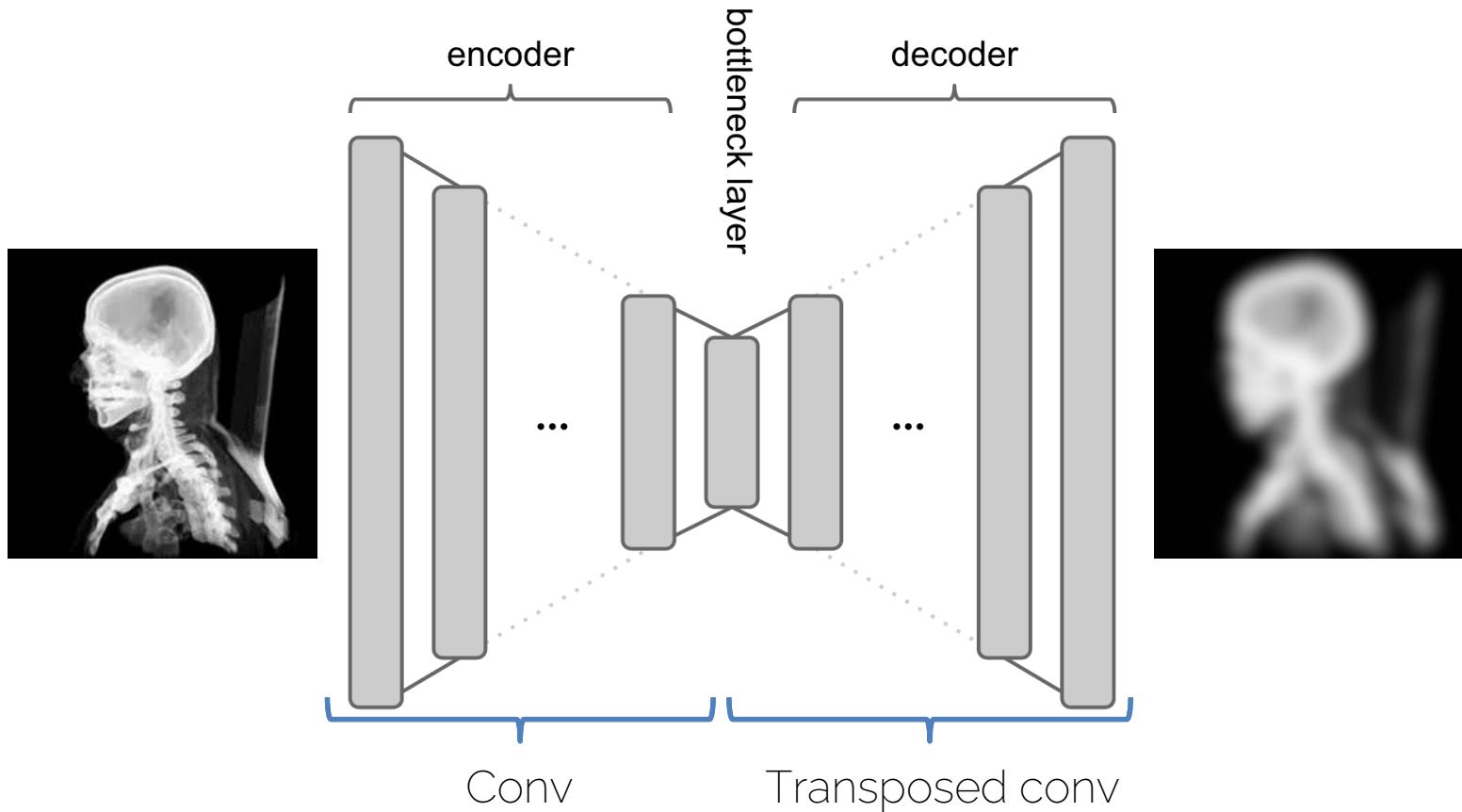
Generative Adversarial Networks (GANs)

Generative Adversarial Networks (GANs)



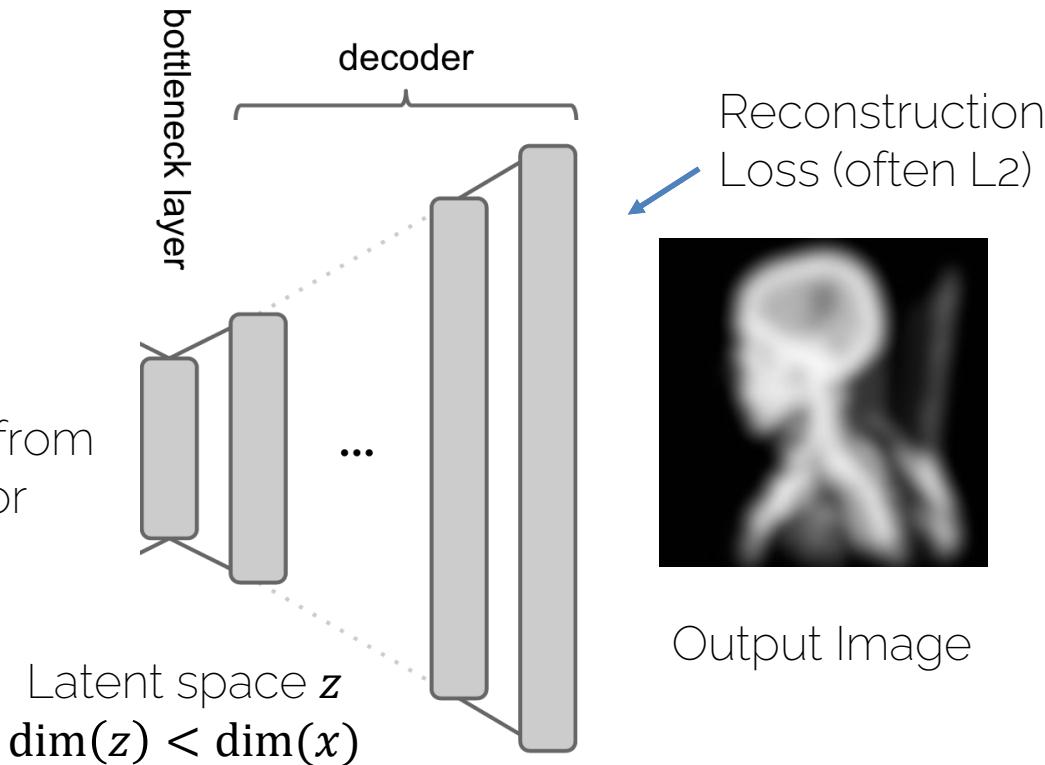
Source: <https://github.com/hindupuravinash/the-gan-zoo>

Autoencoder



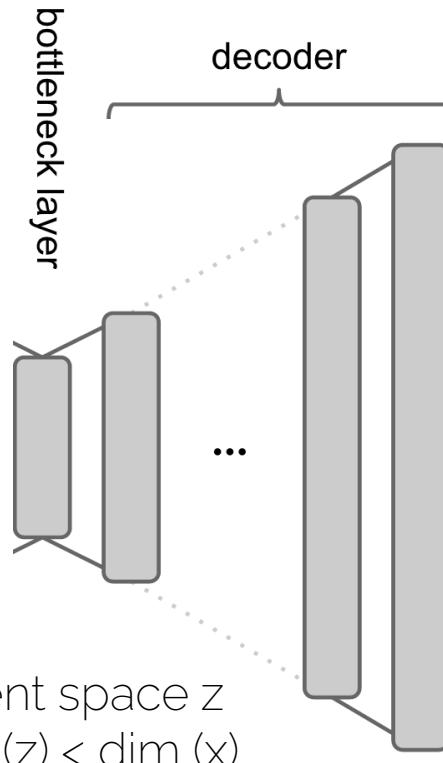
Decoder as Generative Model

Test time:
-> reconstruction from
'random' vector

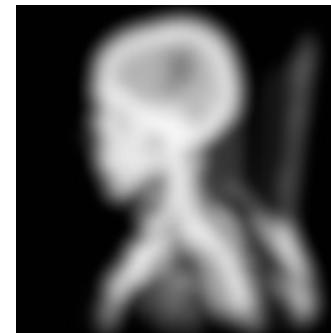


Decoder as Generative Model

"Test time":
-> reconstruction from
'random' vector

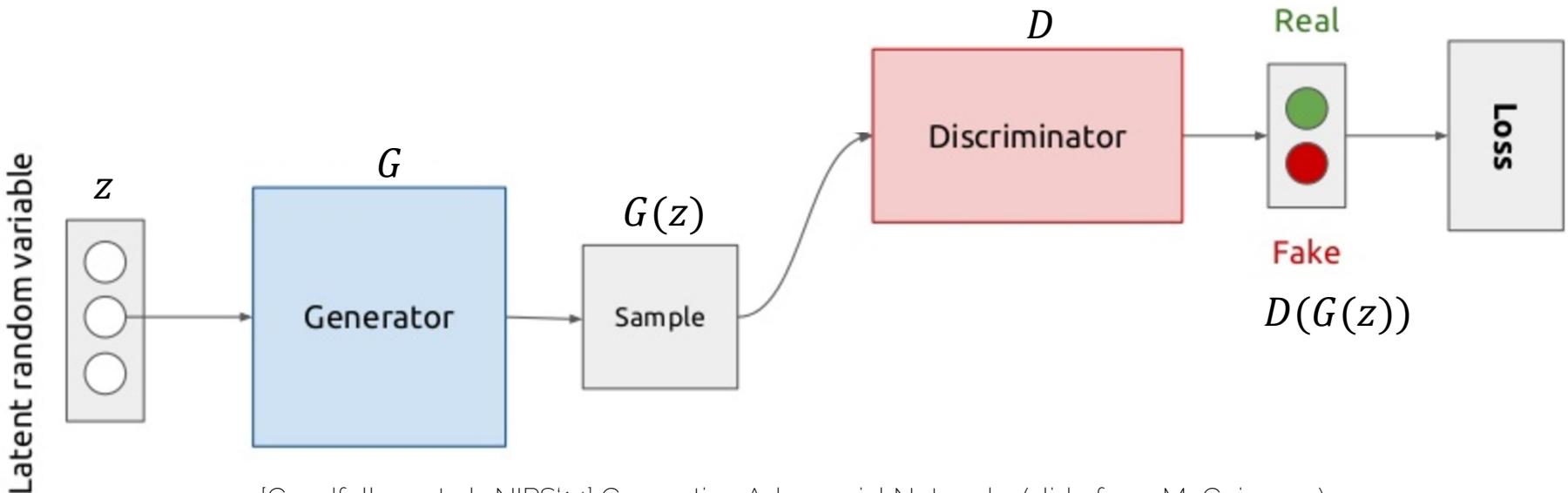


Reconstruction Loss
Often L2, i.e., sum of squared dist.
-> L2 distributes error equally
-> mean is opt.
-> res. is blurry



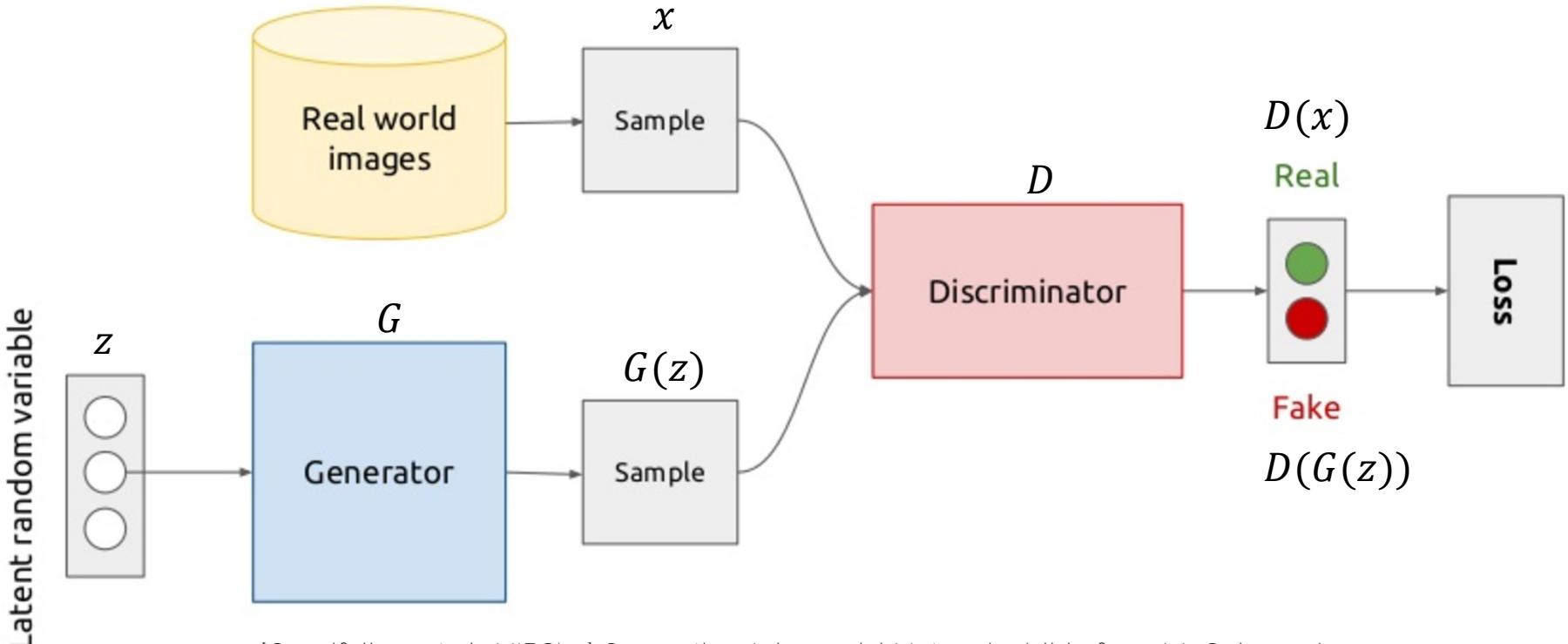
Instead of L2, can we
"learn" a loss function?

Generative Adversarial Networks (GANs)



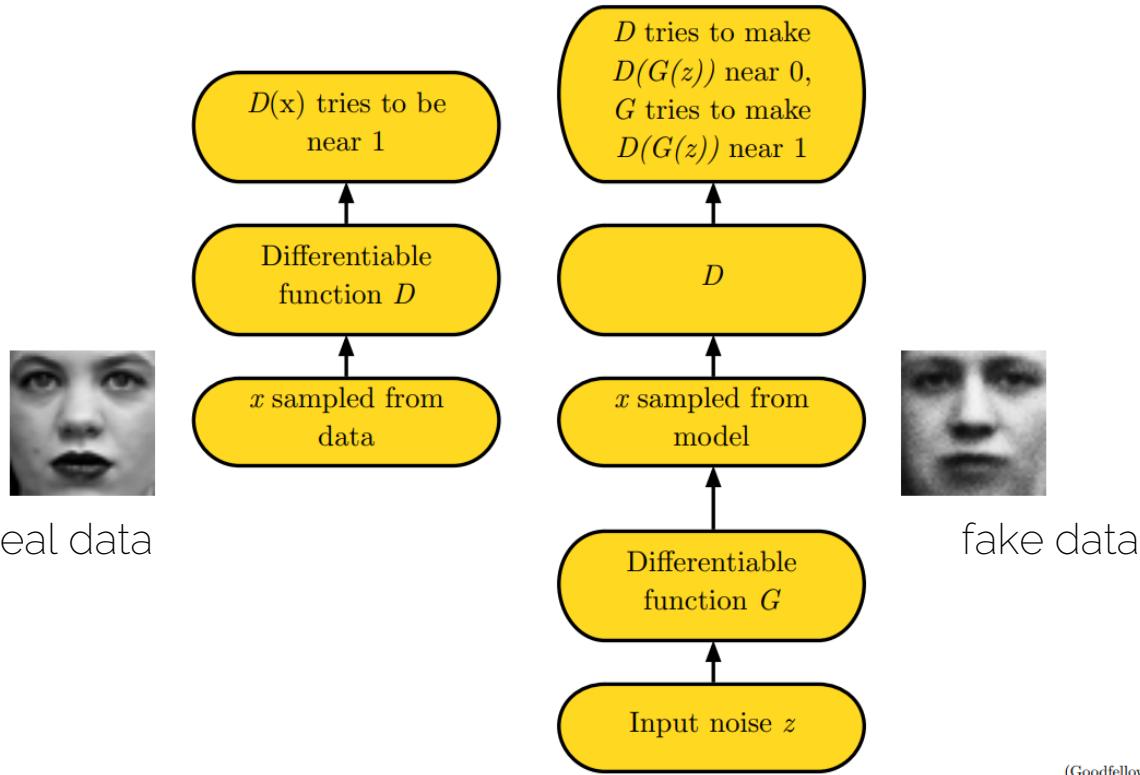
[Goodfellow et al., NIPS'14] Generative Adversarial Networks (slide from McGuinness)

Generative Adversarial Networks (GANs)



[Goodfellow et al., NIPS'14] Generative Adversarial Networks (slide from McGuinness)

Generative Adversarial Networks (GANs)



(Goodfellow 2016)

GANs: Loss Functions

- Discriminator loss

$$J^{(D)} = -\frac{1}{2} \underbrace{\mathbb{E}_{\mathbf{x} \sim p_{data}} \log D(\mathbf{x}) - \frac{1}{2} \mathbb{E}_{\mathbf{z}} \log (1 - D(G(\mathbf{z})))}_{\text{binary cross entropy}}$$

- Generator loss

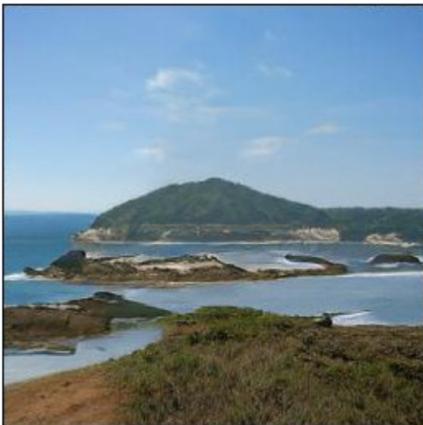
$$J^{(G)} = -J^{(D)}$$

- Minimax Game:

- G minimizes probability that D is correct
 - Equilibrium is saddle point of discriminator loss
 - D provides supervision (i.e., gradients) for G

GAN Applications

BigGAN: HD Image Generation



[Brock et al., ICLR'18] BigGAN : Large Scale GAN Training for High Fidelity Natural Image Synthesis

StyleGAN: Face Image Generation



[Karras et al., '18] StyleGAN : A Style-Based Generator Architecture for Generative Adversarial Networks

[Karras et al., '19] StyleGAN2 : Analyzing and Improving the Image Quality of StyleGAN

Cycle GAN: Unpaired Image-to-Image Translation



Generator
A2B

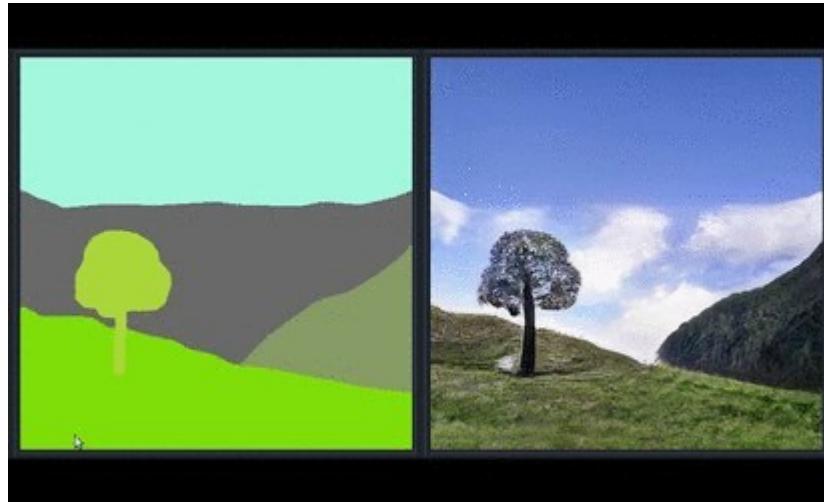


Generator
A2B



[Zhu et al., ICCV'17] Cycle GAN : Unpaired Image-to-Image Translation using Cycle-Consistent Adversarial Networks
I2DL: Prof. Dai

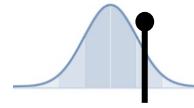
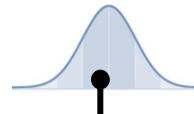
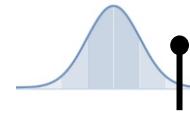
SPADE: GAN-Based Image Editing



[Park et al., CVPR'19] SPADE : Semantic Image Synthesis with Spatially-Adaptive Normalization

I2DL: Prof. Dai

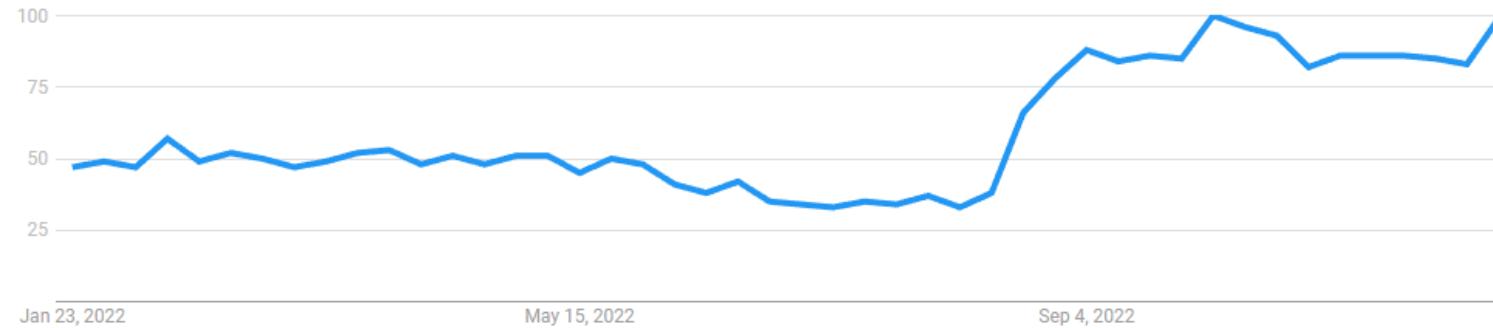
Texturify: 3D Texture Generation

 z_0  z_1  z_2

Diffusion

Diffusion – Search Interest

Interest over time ?



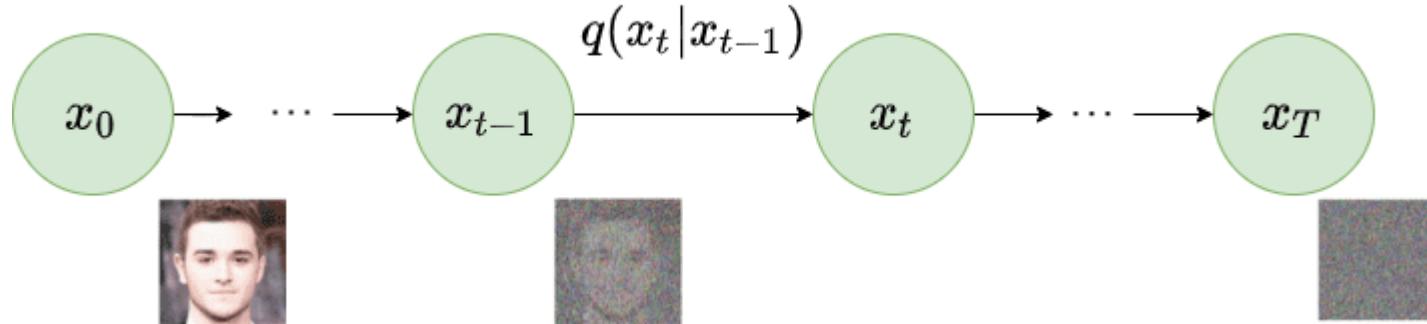
Source: Google Trends

Diffusion Models

- Class of generative models
- Achieved state-of-the-art image generation (DALLE-2, Imagen, StableDiffusion)
- What is diffusion?

Diffusion Process

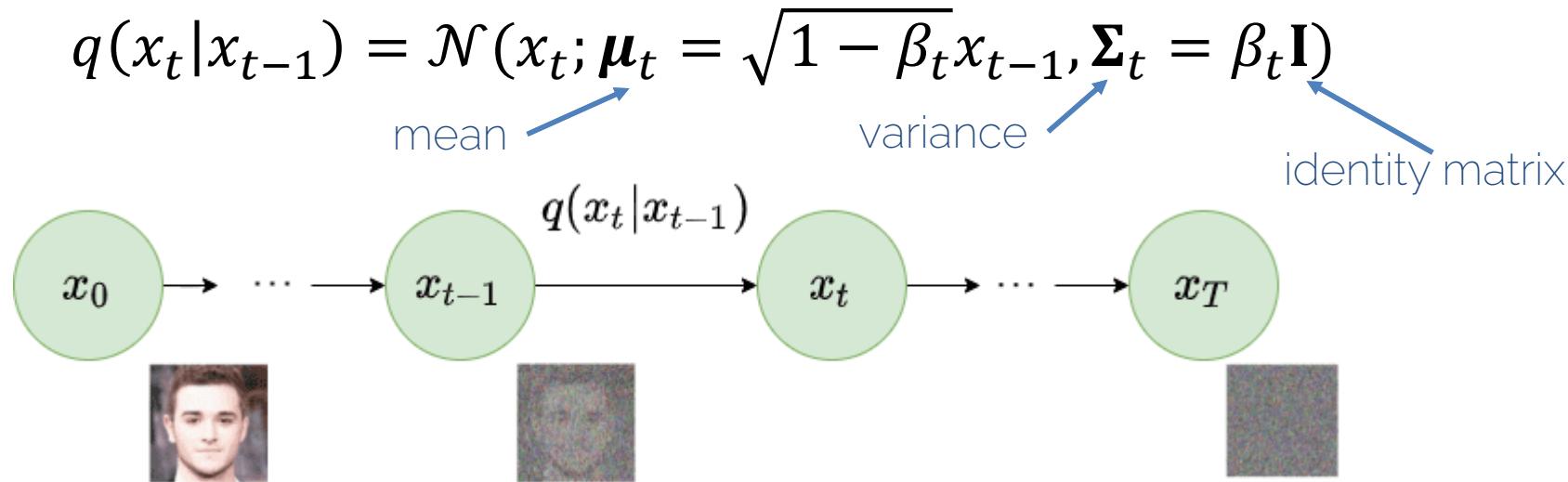
- Gradually add noise to input image x_0 in a series of T time steps
- Neural network trained to recover original data



[Ho et al. '20] Denoising Diffusion Probabilistic Models

Forward Diffusion

- Markov chain of T steps
 - Each step depends only on previous
- Adds noise to x_0 sampled from real distribution $q(x)$



[Ho et al. '20] Denoising Diffusion Probabilistic Models

Forward Diffusion

- Go from x_0 to x_T :

$$q(x_{1:T}|x_0) = \prod_{t=1}^T q(x_t|x_{t-1})$$

- Efficiency?

Reparameterization

- Define $\alpha_t = 1 - \beta_t$, $\overline{\alpha}_t = \prod_{s=0}^t \alpha_s$, $\epsilon_0, \dots, \epsilon_{t-1} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

$$\begin{aligned}x_t &= \sqrt{1 - \beta_t} x_{t-1} + \sqrt{\beta_t} \epsilon_{t-1} \\&= \sqrt{\alpha_t} x_{t-2} + \sqrt{1 - \alpha_t} \epsilon_{t-2} \\&= \dots \\&= \sqrt{\overline{\alpha}_t} x_0 + \sqrt{1 - \overline{\alpha}_t} \epsilon_0\end{aligned}$$

$$x_t \sim q(x_t | x_0) = \mathcal{N}(x_t; \sqrt{\overline{\alpha}_t} x_0, (1 - \overline{\alpha}_t) \mathbf{I})$$

Reverse Diffusion

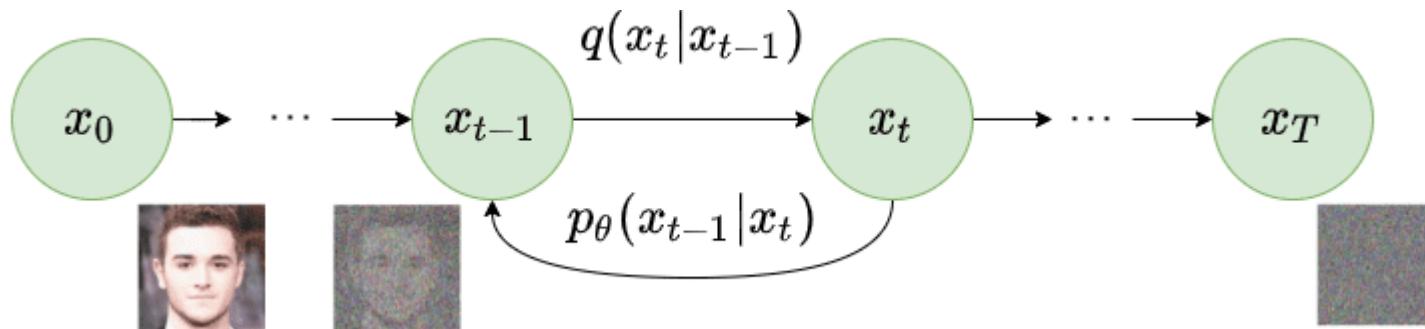
- $x_{T \rightarrow \infty}$ becomes a Gaussian distribution
- Reverse distribution $q(x_{t-1}|x_t)$
 - Sample $x_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ and run reverse process
 - Generates a novel data point from original distribution
- How to model reverse process?

Approximate Reverse Process

- Approximate $q(x_{t-1}|x_t)$ with parameterized model p_θ (e.g., deep network)

$$p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(x_t, t))$$

$$p_\theta(x_{0:T}) = p_\theta(x_T) \prod_{t=1}^T p_\theta(x_{t-1}|x_t)$$



Training a Diffusion Model

- Optimize negative log-likelihood of training data

$$\begin{aligned} L_{VLB} &= \mathbb{E}_q \left[D_{KL}(q(x_T | x_0) || p_\theta(x_T)) \right]_{L_T} \\ &+ \sum_{t=2}^T \underbrace{D_{KL}(q(x_{t-1} | x_t, x_0) || p_\theta(x_{t-1} | x_t))}_{L_{t-1}} - \underbrace{\log p_\theta(x_0 | x_1)}_{L_0} \end{aligned}$$

- Nice derivations: <https://lilianweng.github.io/posts/2021-07-11-diffusion-models>

Training a Diffusion Model

- $L_{t-1} = D_{KL}(q(x_{t-1}|x_t, x_0) || p_\theta(x_{t-1}|x_t))$
- Comparing two Gaussian distributions
- $L_{t-1} \propto \|\tilde{\mu}_t(x_t, x_0) - \mu_\theta(x_t, t)\|^2$
- Predicts diffusion posterior mean

Diffusion Model Architecture

- Input and output dimensions must match
- Highly flexible to architecture design
- Commonly implemented with U-Net architectures

Applications for Diffusion Models

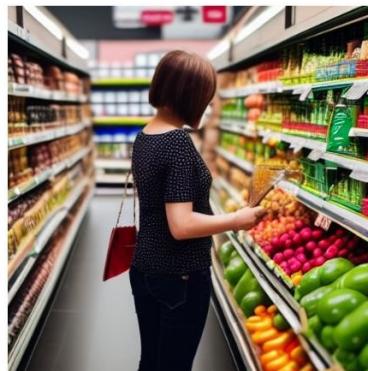
- Text-to-image



Oil Painting



Digital Illustration



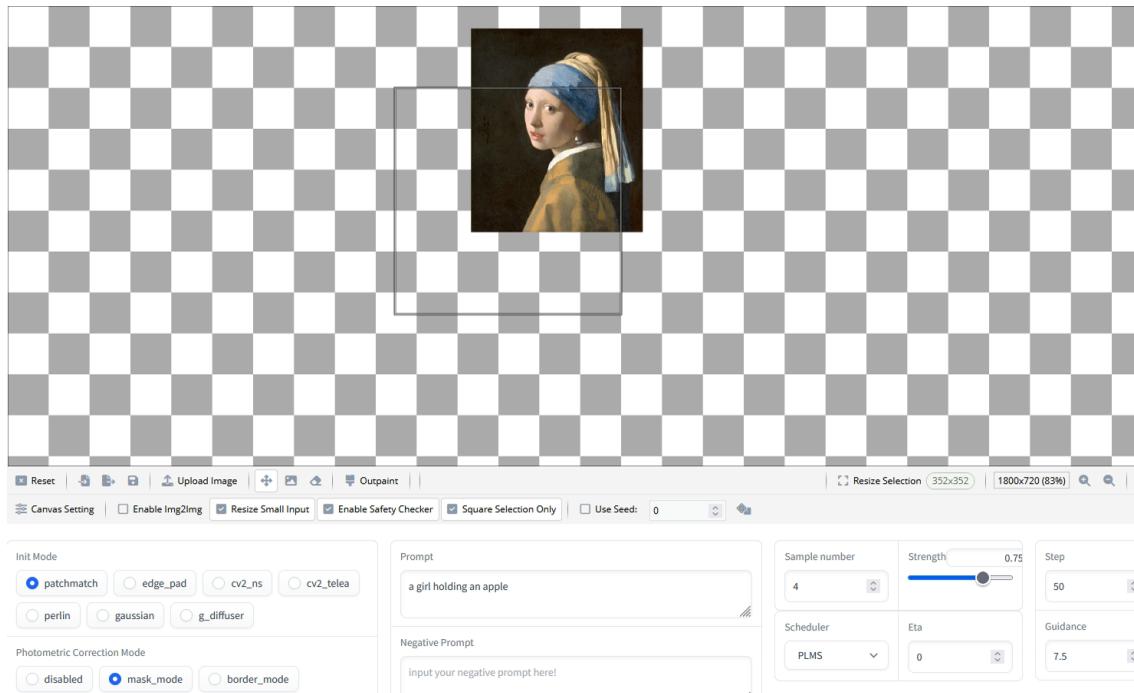
Hyperrealistic



Cartoon

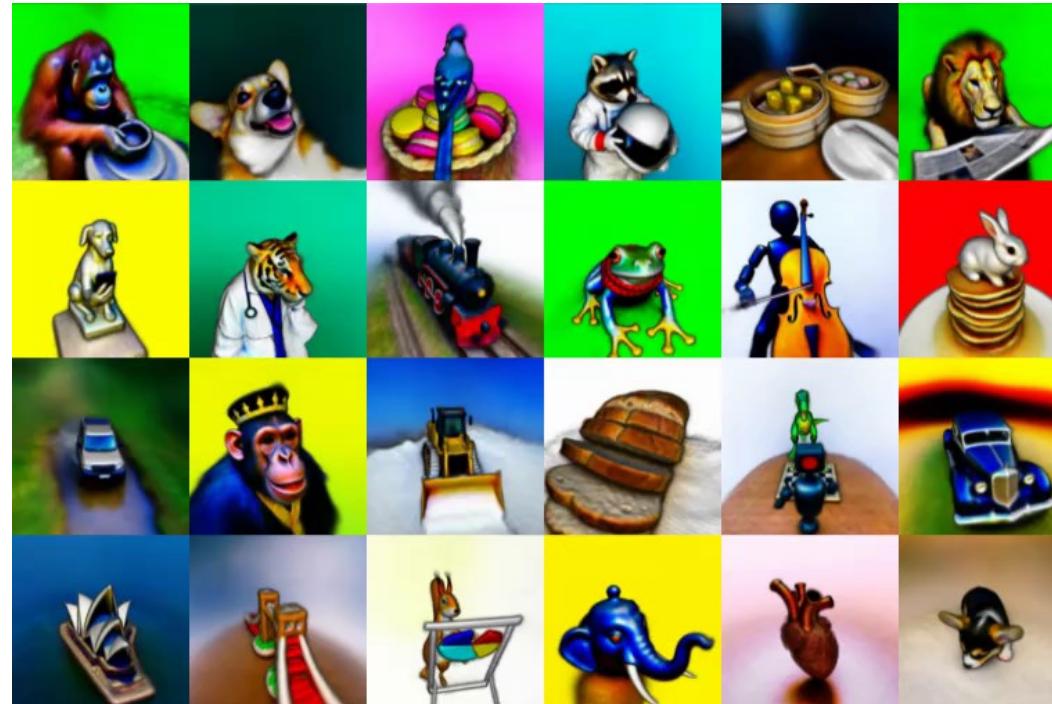
Applications for Diffusion Models

- Image inpainting & outpainting



Applications for Diffusion Models

- Text-to-3D Neural Radiance Fields



Reinforcement Learning

Learning Paradigms in ML

Supervised Learning

E.g., classification,
regression

Labeled data

Find mapping from
input to label

Unsupervised Learning

E.g., clustering,
anomaly detection

Unlabeled data

Find structure in data

Reinforcement Learning

Sequential data

Learning by
interaction with
the environment

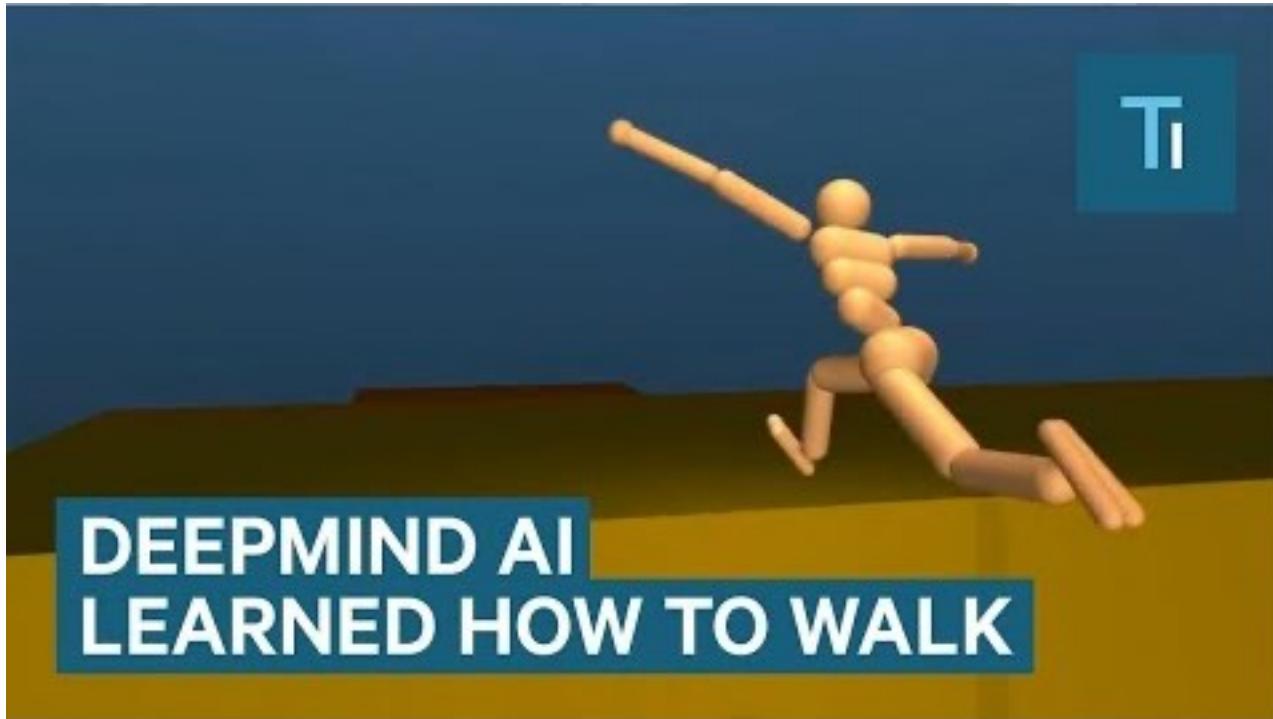
In a Nutshell

- RL-agent is trained using the “carrot and stick” approach
- Good behavior is encouraged by rewards
- Bad behavior is discouraged by punishment



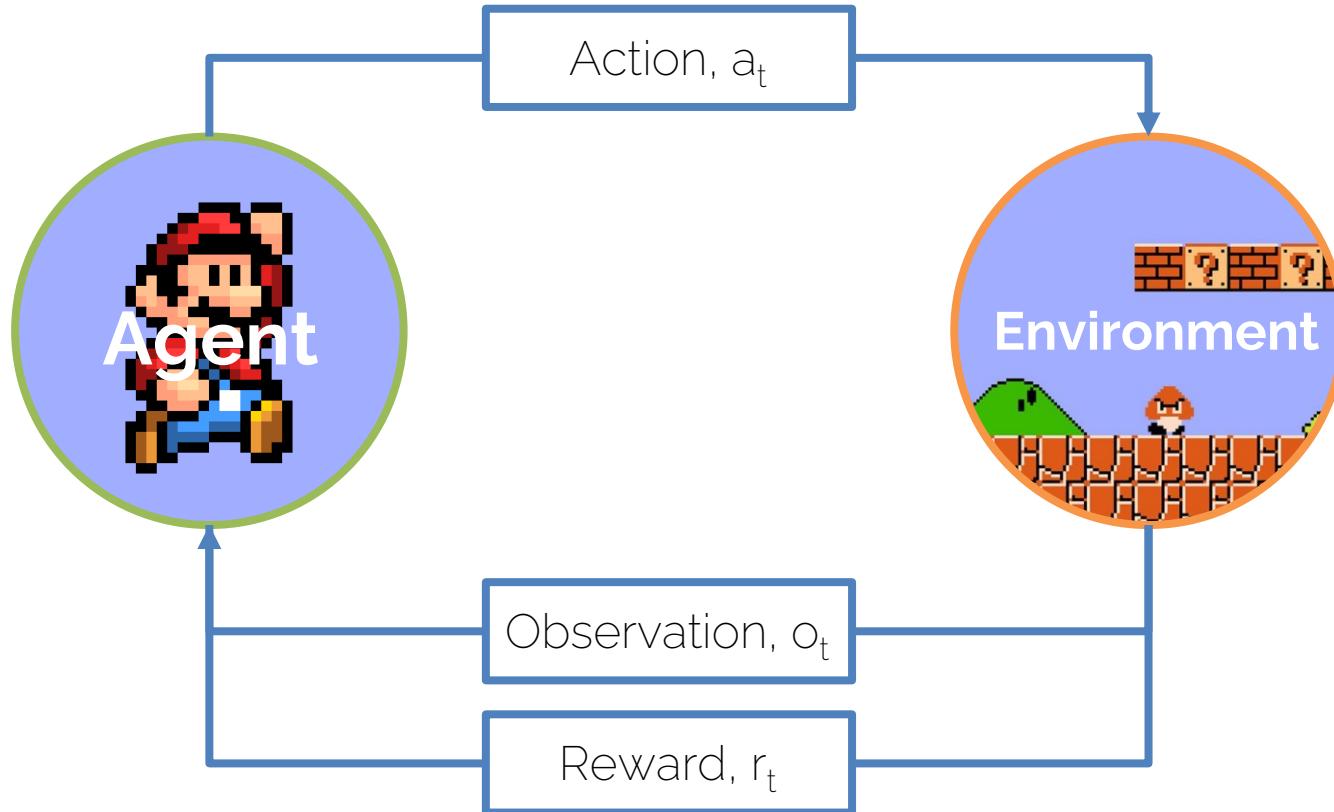
Source: quora.com

Examples of RL: Learning to Walk



Source: Deepmind.com

Agent and Environment



Characteristics of RL

- Sequential, non i.i.d. data (time matters)
- Actions have an effect on the environment
-> Change future input
- No supervisor, target is approximated by the reward signal

History and State

- The agent makes decisions based on the **history h** of observations, actions and rewards up to time-step t

$$h_t = o_1, a_1, r_1, \dots, a_{t-1}, r_{t-1}, o_t$$

- The **state s** contains all the necessary information from $h \rightarrow s$ is a function of h

$$s_t = f(h_t)$$

Markov Assumption

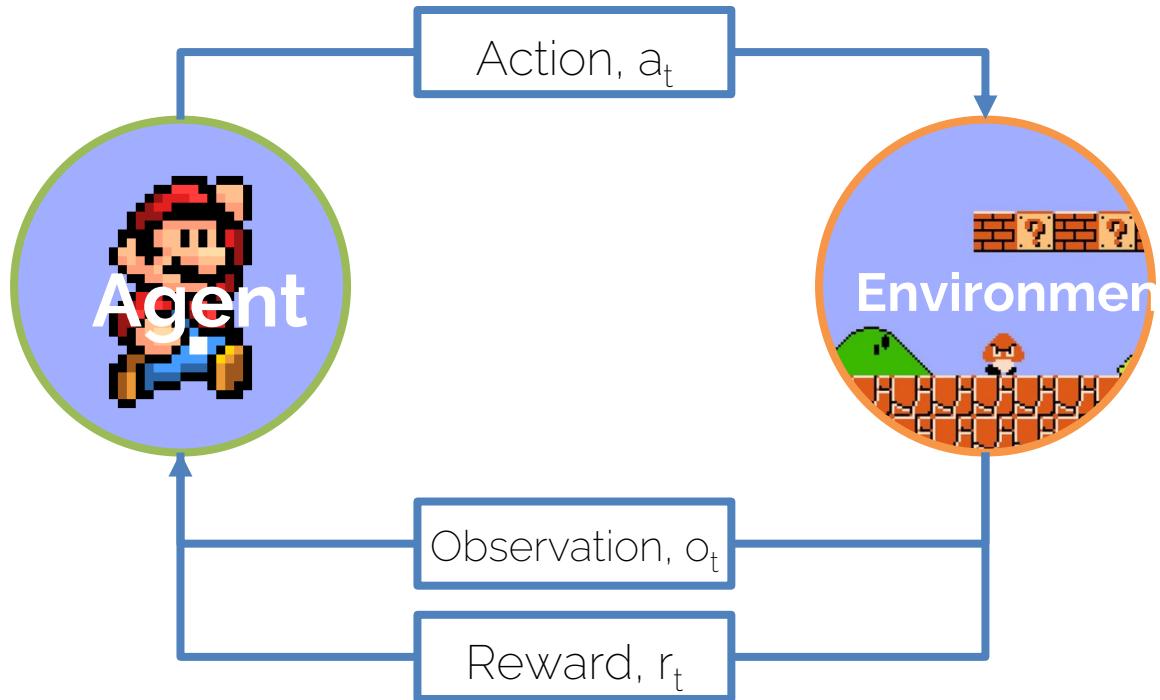
- Problem: History grows linearly over time
- Solution: **Markov Assumption**
- A state S_t is Markov if and only if:

$$\mathbb{P}[s_{t+1}|s_t] = \mathbb{P}[s_{t+1}|s_1, \dots s_t]$$

- “The future is independent of the past given the present”

Agent and Environment

- Reward and next state are functions of current observation o_t and action a_t only



Mathematical Formulation

- The RL problem is a Markov Decision Process (MDP) defined by: $(\mathcal{S}, \mathcal{A}, \mathcal{R}, \mathbb{P}, \gamma)$

\mathcal{S} : Set of possible states

\mathcal{A} : Set of possible actions

\mathcal{R} : Distribution of reward given (state, action) pair

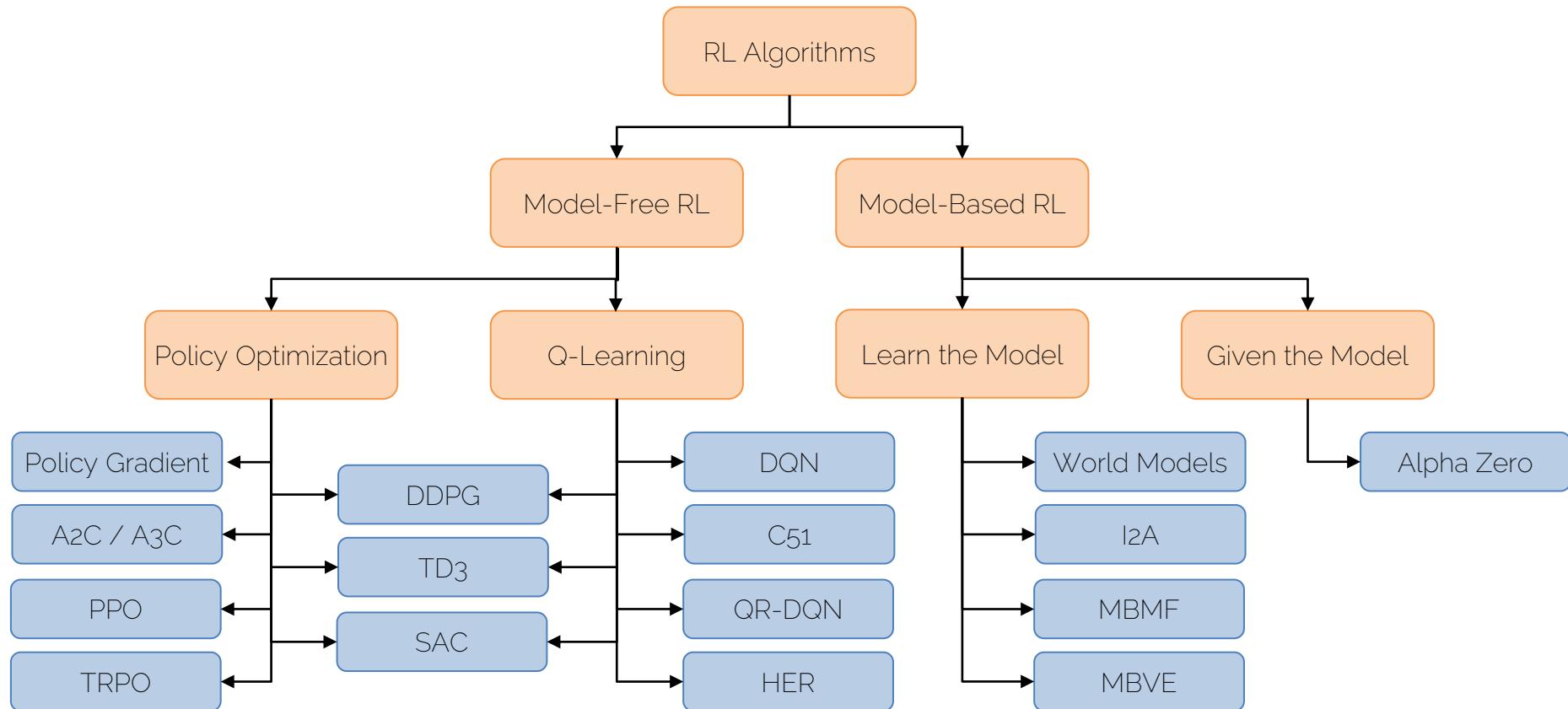
\mathbb{P} : Transition probability of a (state, action) pair

γ : Discount factor (discounts future rewards)

Components of an RL Agent

- Policy π : Behavior of the agent
-> Mapping from state to action: $a = \pi(s)$
- Value-, Q-Function: How good is a state or (state, action) pair
-> Expected future reward

Taxonomy of RL Algorithms



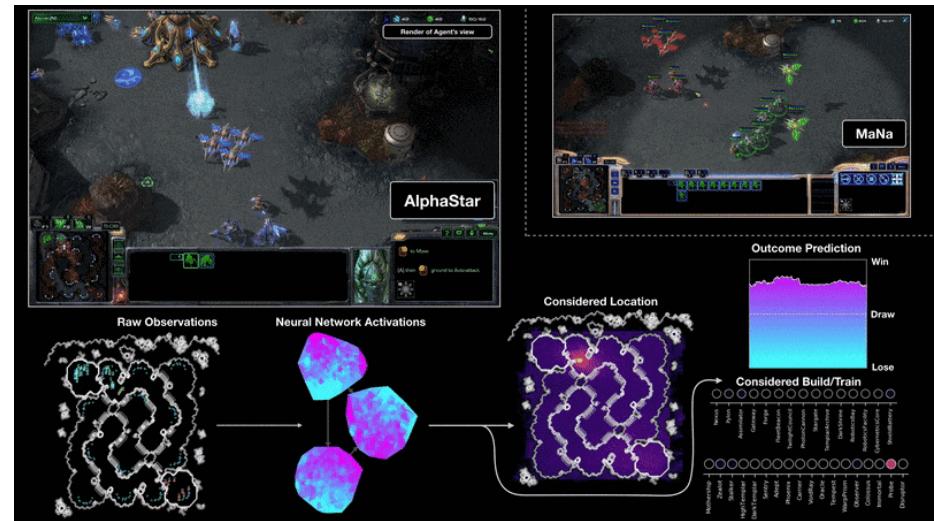
RL Milestones: Playing Atari



- Mnih et al. 2013, first appearance of DQN
- Successfully learned to play different Atari games like Pong, Breakout, Space Invaders, Seaquest and Beam Rider

RL Milestones: AlphaZero (StarCraft)

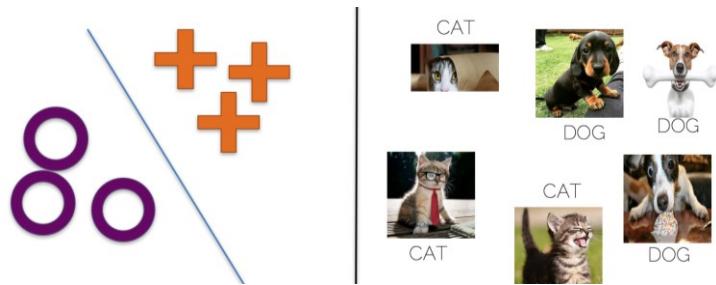
- Model: Transformer network with a LSTM core
- Trained on 200 years of StarCraft play for 14 days
- 16 Google v3 TPUs
- December 2018:
Beats MaNa, a professional StarCraft player (world rank 13)



I2DL Overview

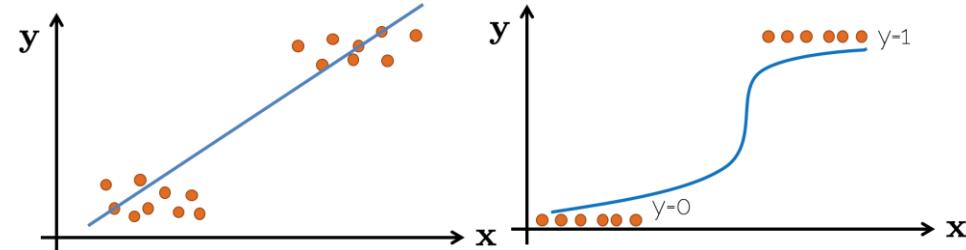
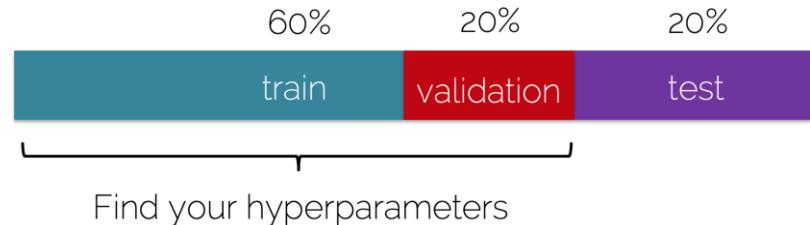
Machine Learning Basics

- Unsupervised vs Supervised Learning



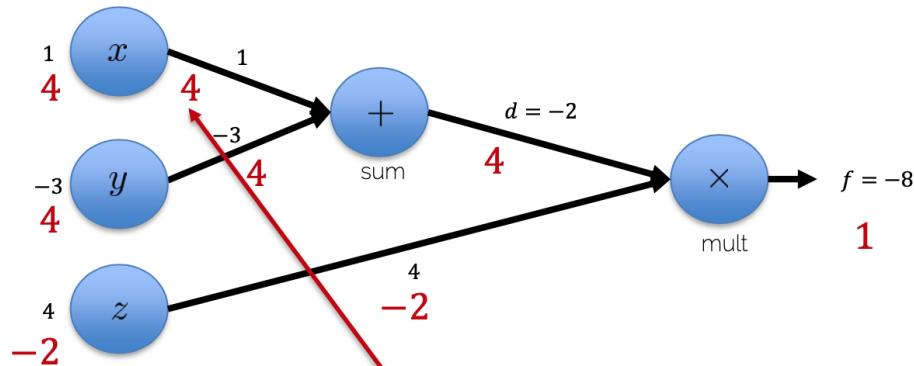
- Linear vs logistic regression

- Data splitting



Intro to Neural Networks

- Backpropagation

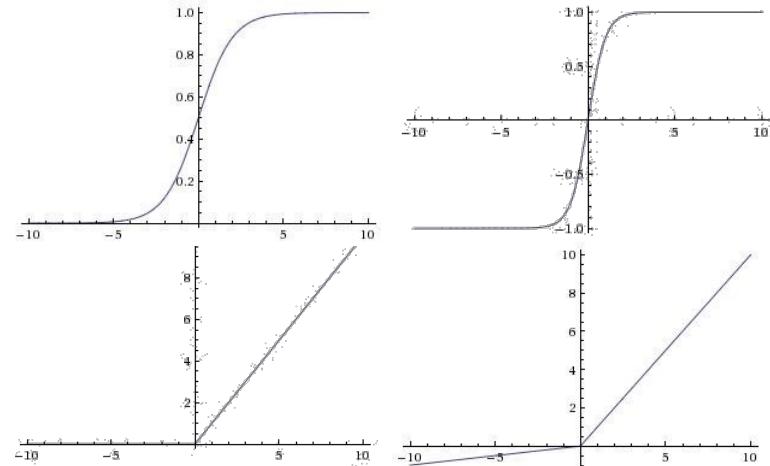


Chain Rule:

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial d} \cdot \frac{\partial d}{\partial x}$$

$$\boxed{\frac{\partial f}{\partial x}}$$

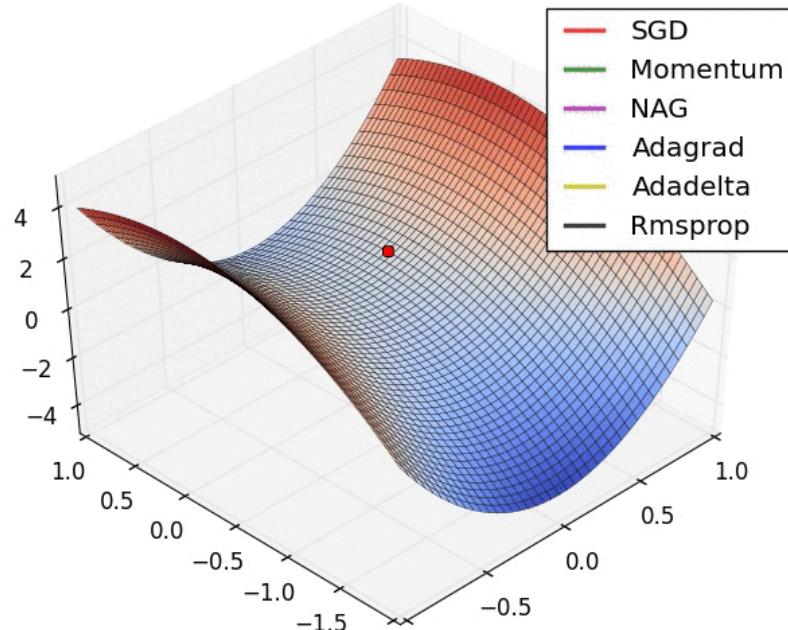
- Activation functions



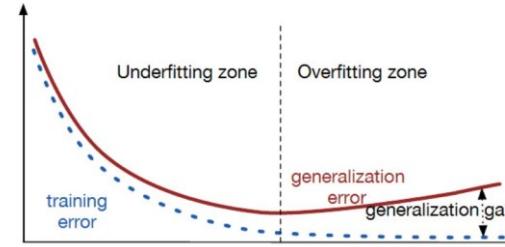
- Loss functions
 - Comparison & effects

Training Neural Networks

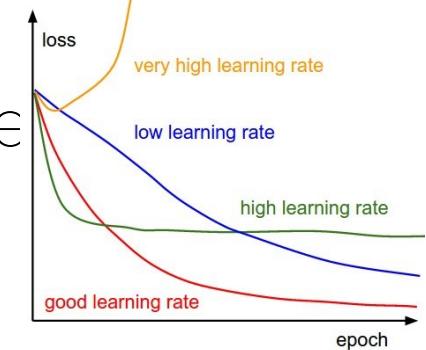
- Gradient Descent/ SGD



- Regularization



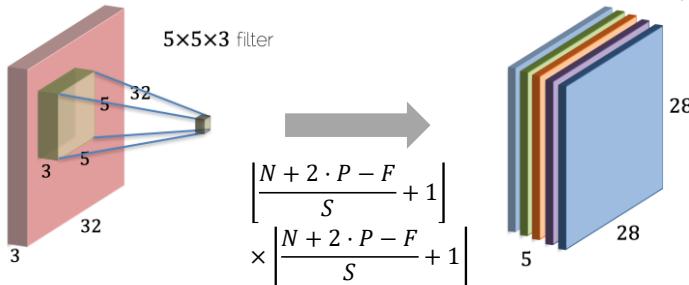
- Parameter & interpretation



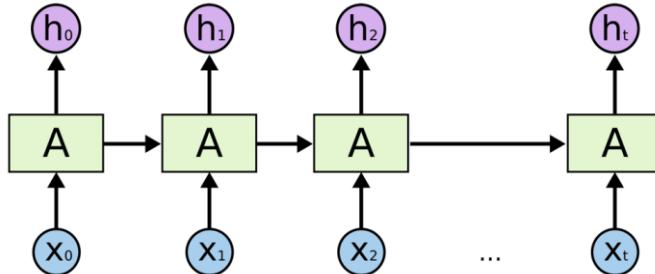
Source: <http://ruder.io/optimizing-gradient-descent/>,
<https://srdas.github.io/DLBook/ImprovingModelGeneralization.html>,
<http://cs231n.github.io/neural-networks-3/>

Typology of Neural Networks

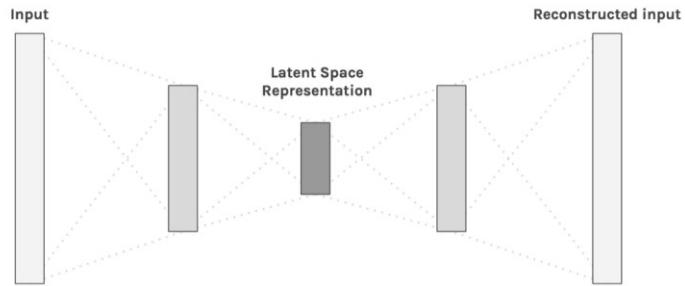
- CNNs



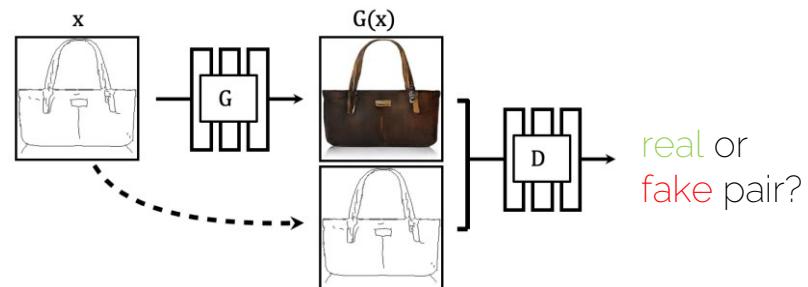
- RNNs



- Autoencoder

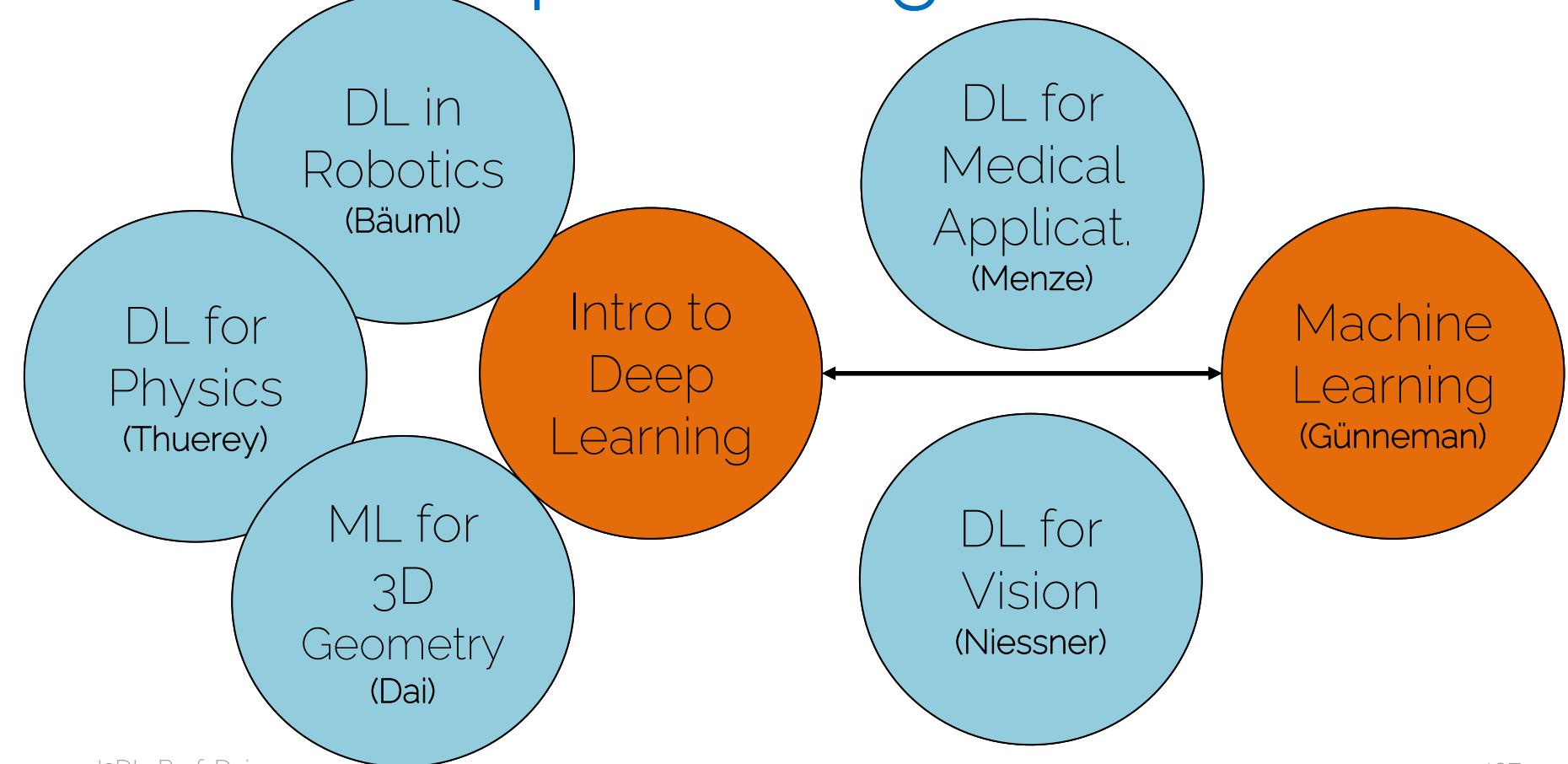


- GANs



Other DL Courses

Deep Learning at TUM



Deep Learning at TUM

- Keep expanding the courses on Deep Learning
- This Introduction to Deep Learning course is the basis for a series of Advanced DL lectures on different topics
- Advanced topics are only for Master students
 - Preparation for MA theses, etc.

Advanced DL for Computer Vision

- Deep Learning for Vision (Profs. Niessner)
- Syllabus
 - Advanced architectures, e.g., Siamese neural networks
 - Variational Autoencoders
 - Generative models, e.g. GAN,
 - Multi-dimensional CNN
 - Graph neural networks
 - Domain adaptation

Advanced DL for Computer Vision

- Deep Learning for Vision
 - 2 V + 3 P
 - Must have attended the Intro to DL
 - Practical part is a project that will last the whole semester
 - Please do not sign up unless you are willing to spend a lot of time on the project!

ML for 3D Geometry

- Lectures + Practical Project
 - Geometric foundations
 - Shape descriptors, similarity, segmentation
 - Shape modeling, reconstruction, synthesis
 - Deep learning for multi-view, volumetric, point cloud, and graph data
 - Prof. Dai

Next Dates and Exam

- Friday (31.01): Guest Lecture, Prof. Björn Ommer
 - Here in HS1!
- Exam date: **February 10th** at **18:30-20:00**
- There will NOT be a retake exam
- Neither cheat sheet nor calculator during the exam

Good Luck
in the Exam ☺

References for Further Reading

- <https://towardsdatascience.com/intuitively-understanding-variational-autoencoders-1bfe67eb5daf>
- <https://phillipi.github.io/pix2pix/>
- http://cs231n.stanford.edu/slides/2017/cs231n_2017_lecure13.pdf