Data Mining: Artificial Neural Network

Lecture Notes for Chapter 3

Data Mining

https://ml-graph.github.io/winter-2025/

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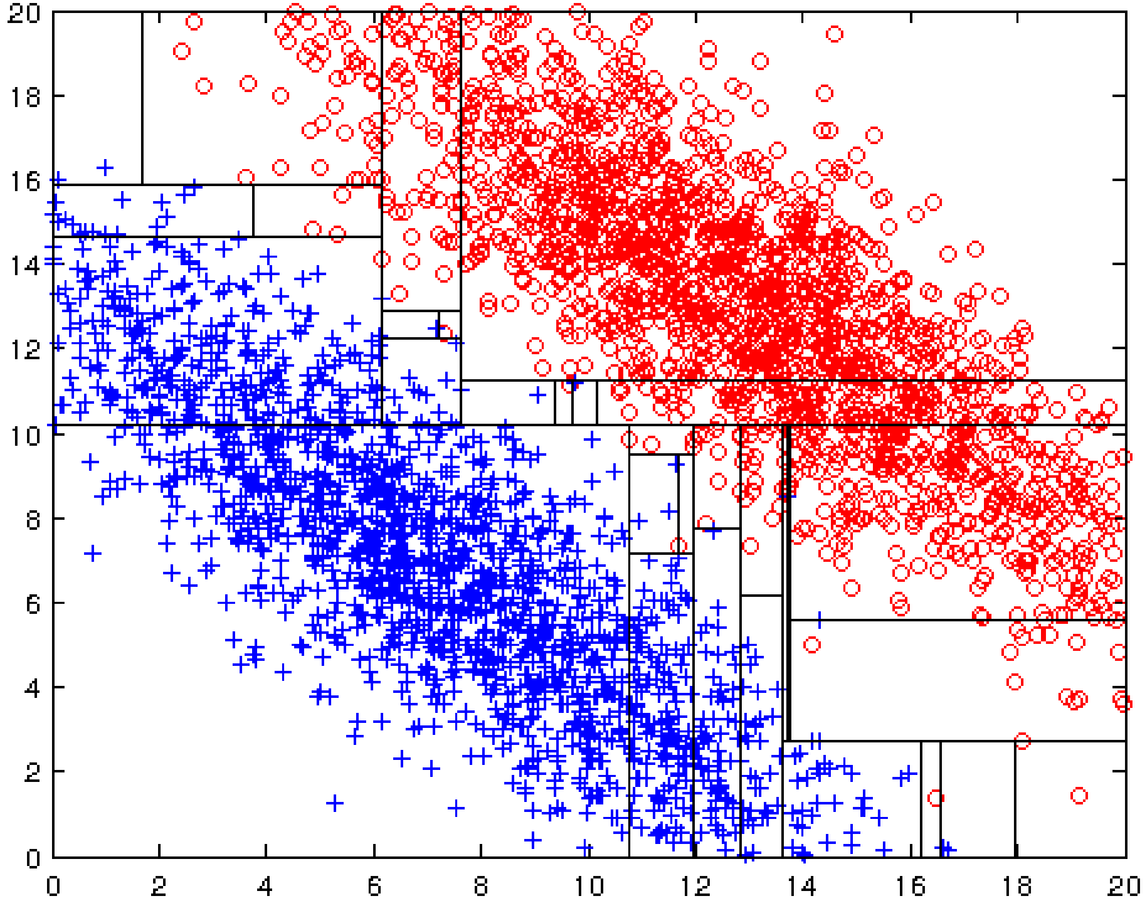
CS 453/553 – Winter 2025

Course Lecture is very heavily based on

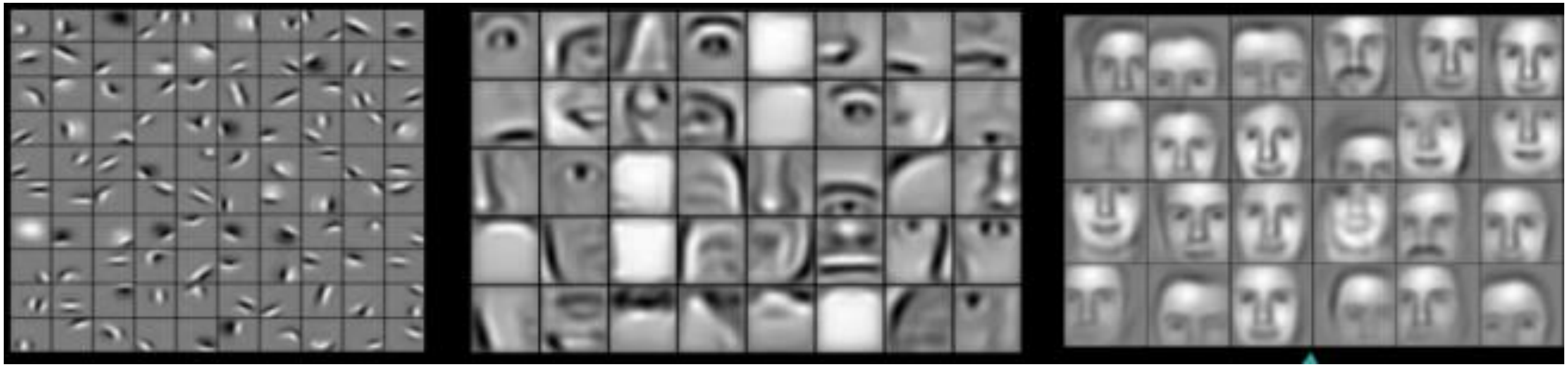
"Introduction to Data Mining"

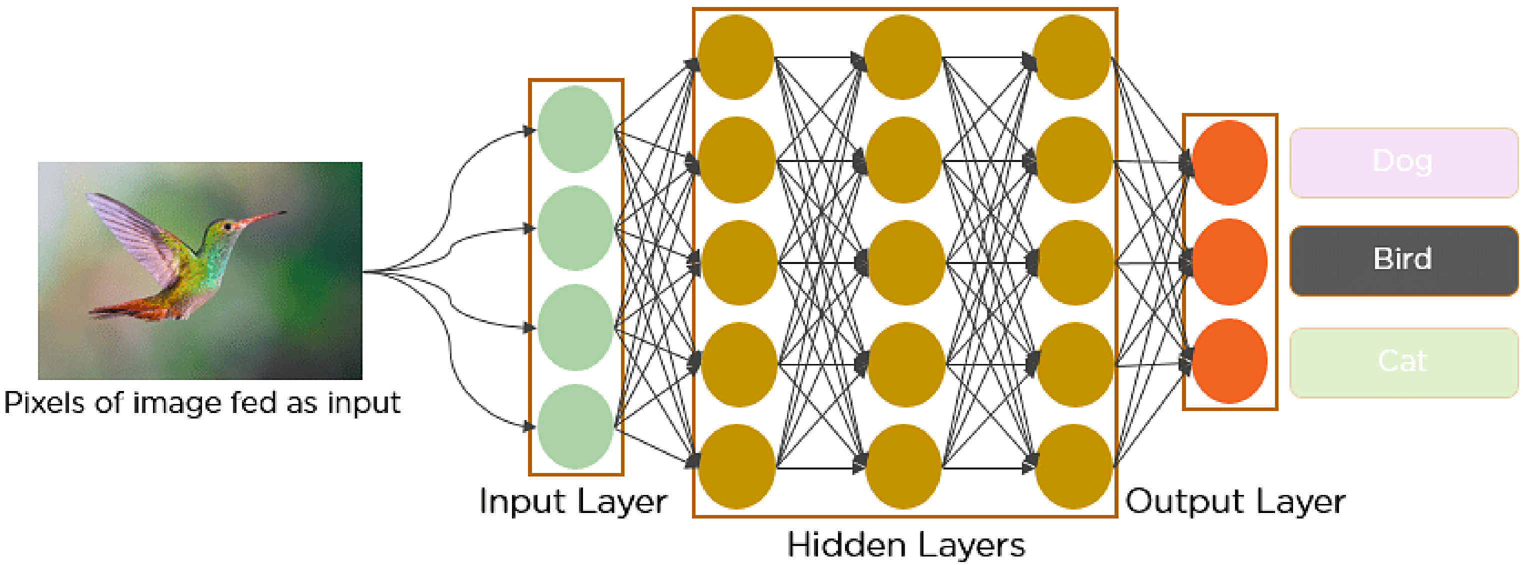
by Tan, Steinbach, Karpatne, Kumar

Limitations of Decision-Tree and many other model

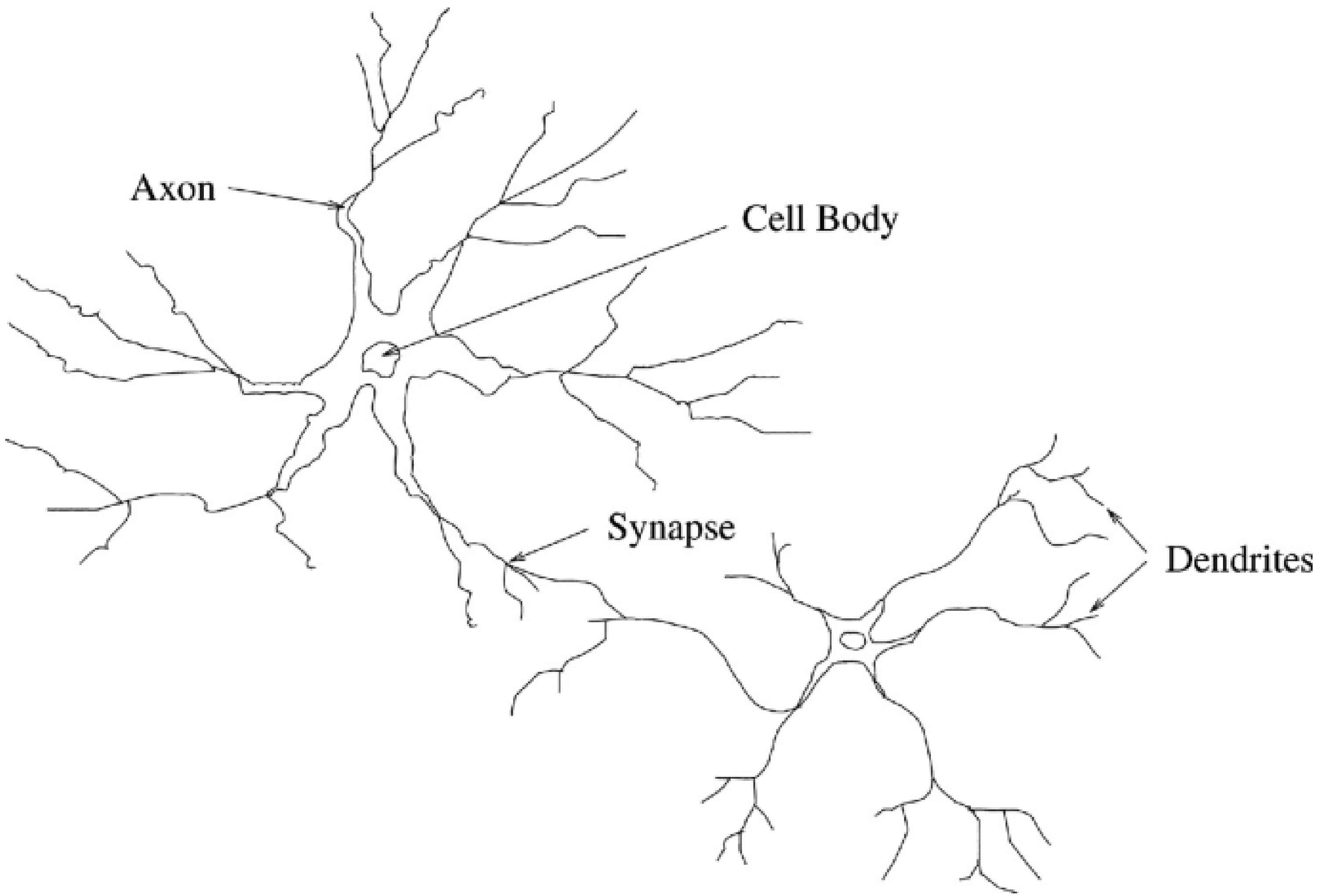


Real-world Intuition





Basic Architecture of Perceptron

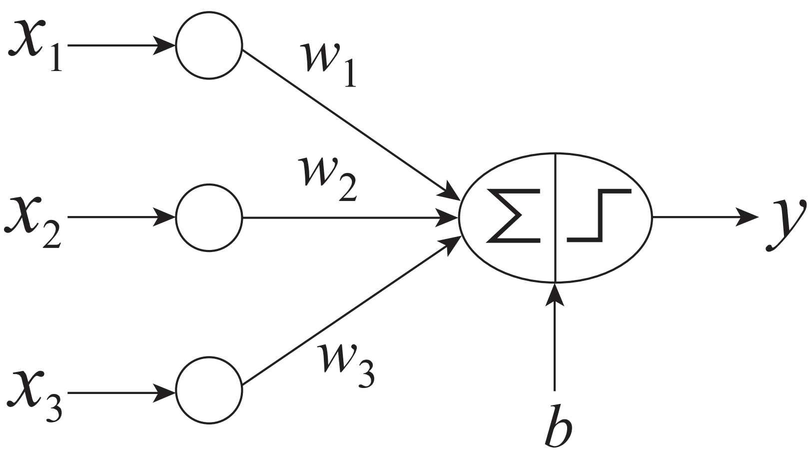


Artificial Neural Networks (ANN)

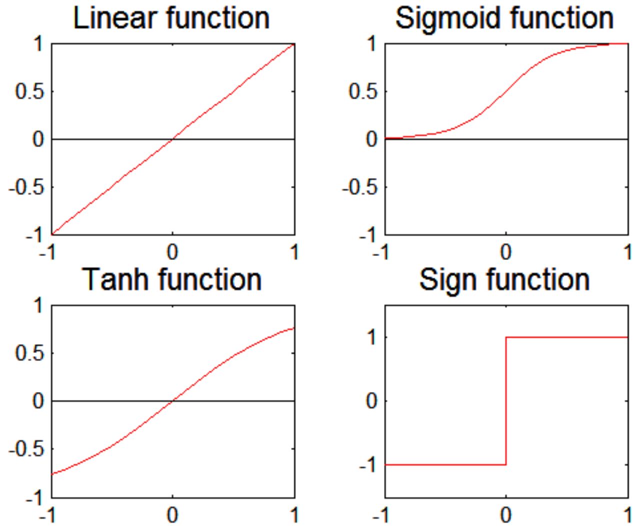
- **Basic Idea: A complex non-linear function can be learned as a composition of simple processing units**

- **ANN is a collection of simple processing units (nodes) that are connected by directed links (edges)**
  - **Every node receives signals from incoming edges, performs computations, and transmits signals to outgoing edges**
  - **Analogous to *human brain* where nodes are neurons and signals are electrical impulses**
  - **Weight of an edge determines the strength of connection between the nodes**
- **Simplest ANN: Perceptron (single neuron)**

Basic Architecture of Perceptron



$$y = \sigma(w^{\mathrm{T}}x + b)$$



What happens if there is no nonlinear activation?

Linear Regression

- Data - $\left\{\left(x^{(i)}, y^{(i)}\right)\right\}_{i=1}^{N}$

$$\text{f(x)} = xw + b$$

- Regression – Find f that minimizes our uncertainty about y given x

$$y = f(x) + n$$

- Minimizing Mean Squared Error = Minimizing Negative Log-Likelihood

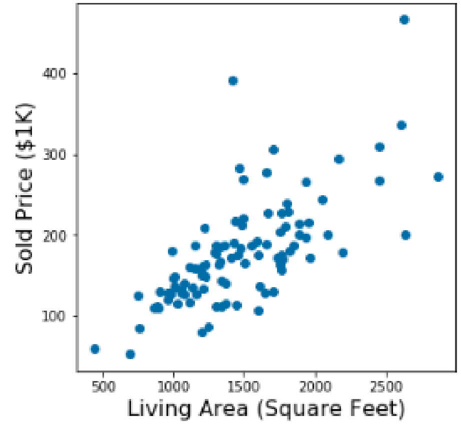
$$\underset{f}{\operatorname{argmin}} \frac{1}{N} \sum_{i=1}^{N} \left(y^{(i)} - f\left(x^{(i)}\right)\right)^2$$

Linear Regression

$$\underset{w}{\operatorname{argmin}} \boxed{\frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - w^T\hat{x}^{(i)}\right)^2} = \underset{w}{\operatorname{argmin}} \boxed{\frac{1}{N}\|y - Xw\|^2}$$

Loss/Cost Function

$$\underset{f}{\operatorname{argmin}} \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - f\left(x^{(i)}\right)\right)^2$$



Where

- $y = \left[y^{(1)}, \dots, y^{(N)}\right]^T \in \mathbb{R}^{N\times 1}$ and
- $X = \left[\hat{x}^{(1)}, \dots, \hat{x}^{(N)}\right]^T \in \mathbb{R}^{N\times(d+1)}$ (here $d = 1$)
- $w = [w_0, w_1, \dots, w_d]^{\mathrm{T}} \in \mathbb{R}^{d+1}$

Linear Regression

$$J(w) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - w^T\hat{x}^{(i)}\right)^2$$

Compute the minimum value? How to do it in Math?

Find points where gradient = 0

Linear Regression

$$J(w) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - w^T\hat{x}^{(i)}\right)^2$$

$$J(W) = \frac{1}{N}(Y - XW)^T(Y - XW)$$

https://www.math.uwaterloo.ca/~hwolkowi/matrixcookbook.pdf

$$J(W) = \frac{1}{N}\left(Y^TY - 2Y^TXW + W^TX^TXW\right)$$

$$\nabla J(W) = \frac{\partial}{\partial W}\left[\frac{1}{N}(Y^TY - 2Y^TXW + W^TX^TXW)\right]$$

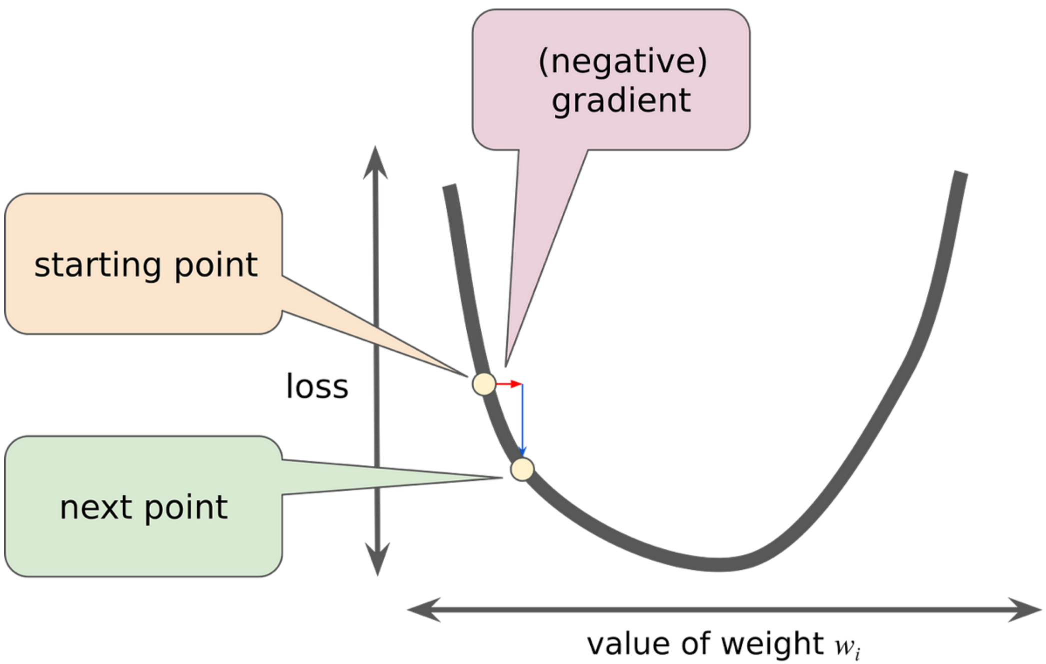
$$X^TXW = X^TY$$

$$W^* = (X^TX)^{-1}X^TY$$

$$\nabla J(W) = -\frac{2}{N}X^TY + \frac{2}{N}X^TXW$$

Linear Regression

$$J(w) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - w^T\hat{x}^{(i)}\right)^2$$



If the gradient of a function is non-zero at a point, the direction of the gradient is the direction in which the function increases most quickly

Linear Regression

$$J(w) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - w^T\hat{x}^{(i)}\right)^2$$

$$\nabla J(w) = \frac{\partial J(w)}{\partial w}$$

$$J(w) = \frac{1}{N}\sum_{i=1}^{N}(y^{(i)} - w^T\hat{x}^{(i)})^2$$

$$\frac{\partial J(w)}{\partial w} = \frac{1}{N}\sum_{i=1}^{N}2(y^{(i)} - w^T\hat{x}^{(i)})(-\hat{x}^{(i)})$$

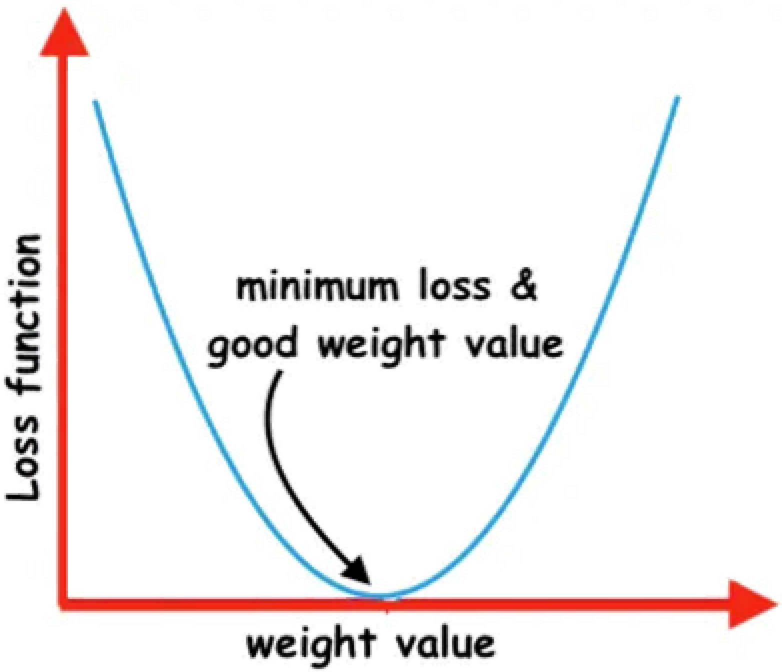
$$= -\frac{2}{N}\sum_{i=1}^{N}(y^{(i)} - w^T\hat{x}^{(i)})\hat{x}^{(i)}$$

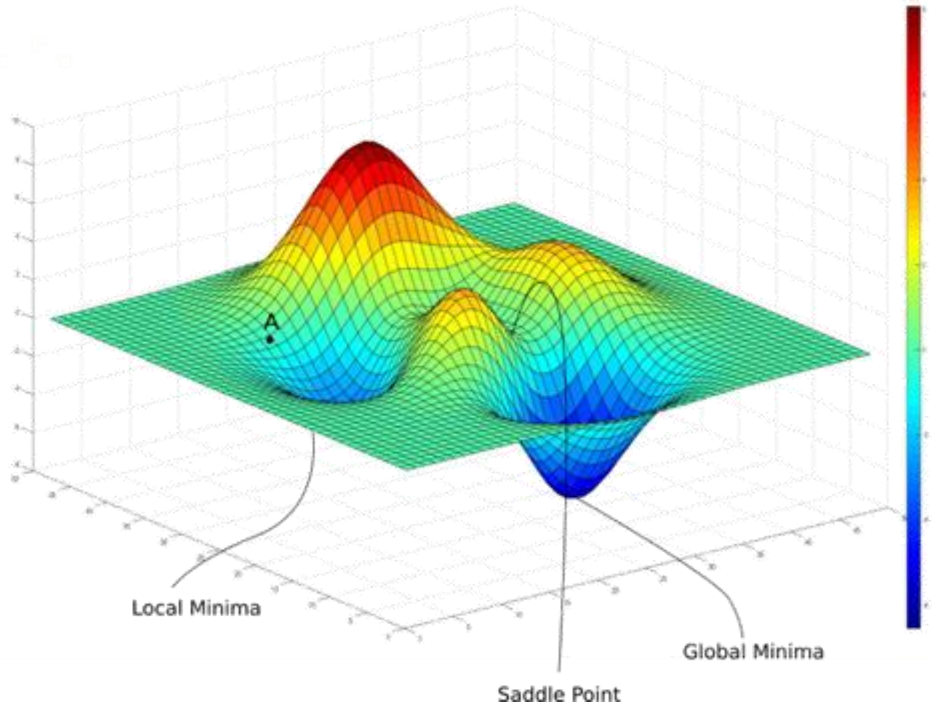
$$\nabla J(w) = -\frac{2}{N}\sum_{i=1}^{N}(y^{(i)} - w^T\hat{x}^{(i)})\hat{x}^{(i)}$$

$$w_0 := w_0 + \frac{2\alpha}{N}\sum_{i=1}^{N}(y^{(i)} - (w_0 + w_1x_1^{(i)}))$$

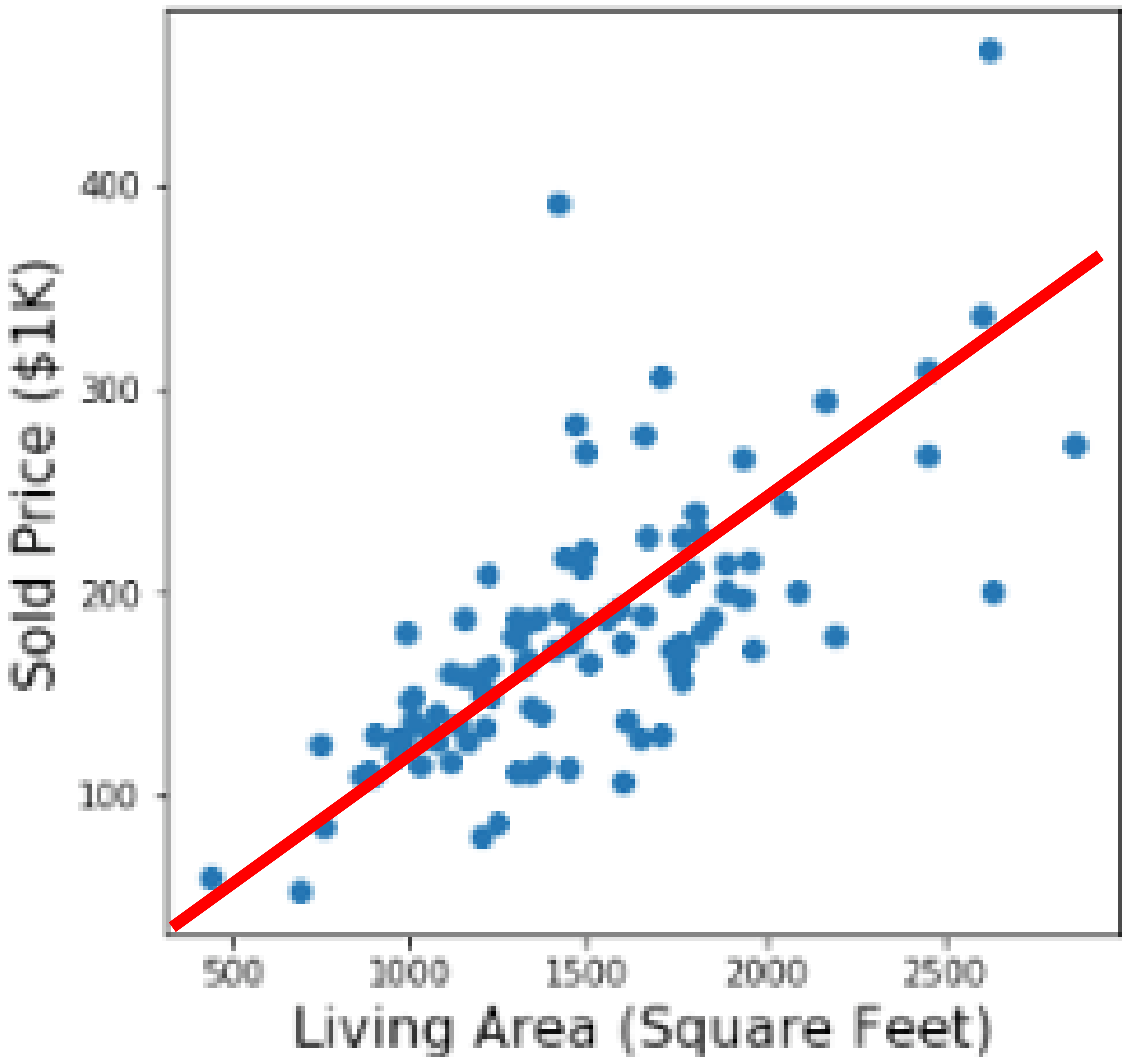
$$w_1 := w_1 + \frac{2\alpha}{N}\sum_{i=1}^{N}(y^{(i)} - (w_0 + w_1x_1^{(i)}))x_1^{(i)}$$

Local Minimum vs Global Minimum





Linear Regression

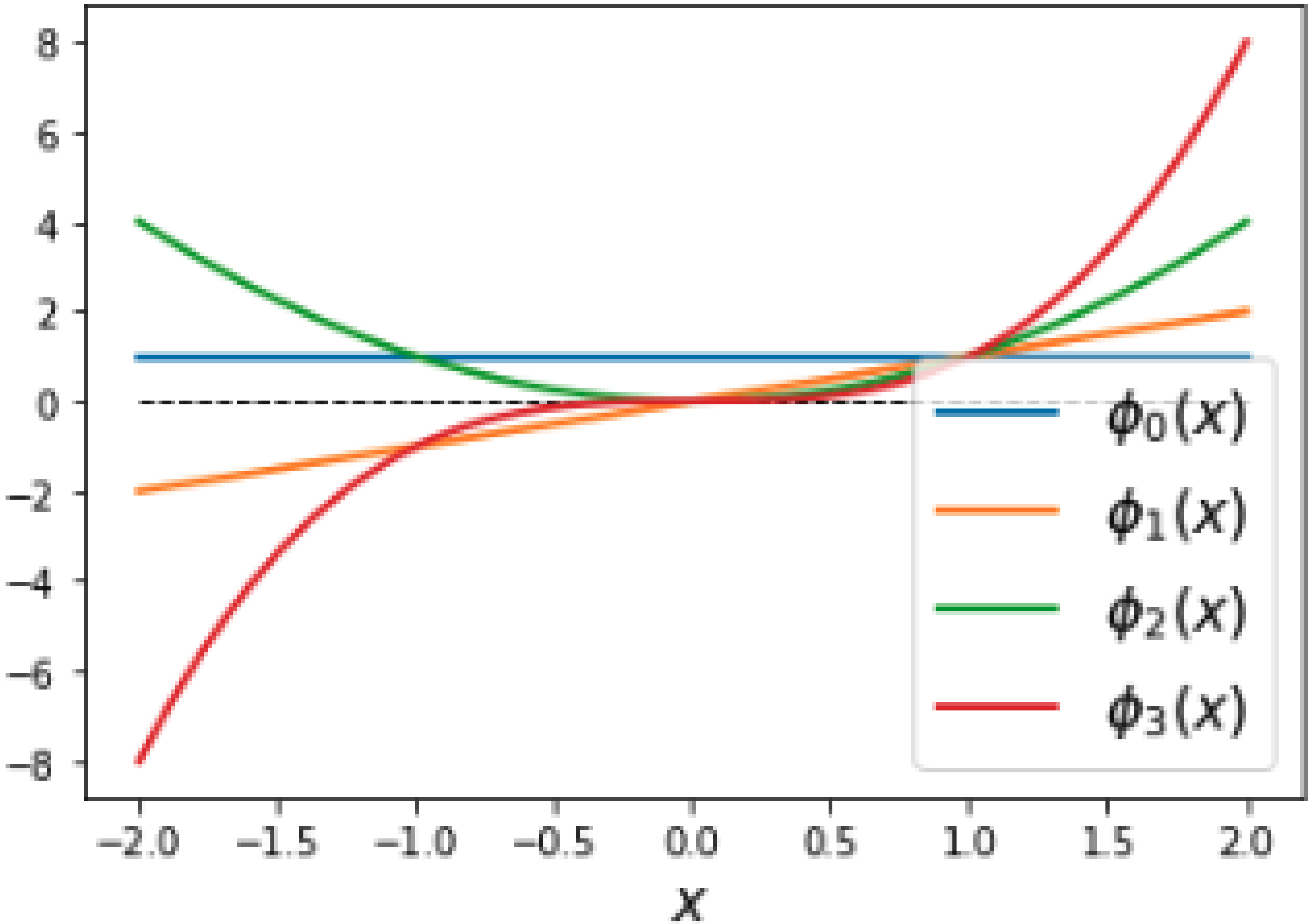


$$f(x) = w_0 x + b$$

Slope

Intercept

Problem of Linear Regression



NonLinear Regression

- So far, we have been using a linear function for regression:

$$f(x) = w^T x + w_0 = \sum_{i=0}^{d} w_i x_i \quad \text{(Assuming } x_0 = 1\text{)}$$

- Lets generalize this model:

$$f(x) = \sum_{i=0}^{M} w_i \phi_i(x) = w^T \phi(x)$$

where ϕ_i are fixed “basis” functions.

- For linear regression $M = d$, $\phi_i(x) = x_i$.

NonLinear Regression

$$f(x) = \sum_{i=0}^{M} w_i \phi_i(x) = w^T \phi(x)$$

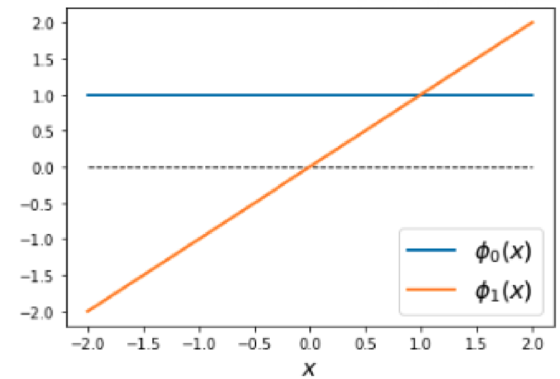
E.g., Polynomial Regression:

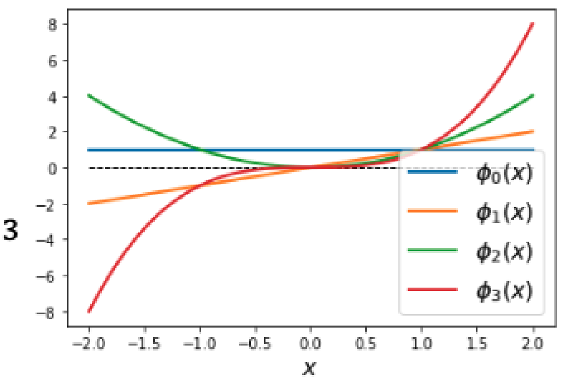
- 1D Polynomial Regression, $\phi(x) = [1, x, x^2, x^3]$:

$$\underset{w}{\operatorname{argmin}} \frac{1}{N} \sum_{n=1}^{N} \left(w^T \phi\left(x^{(i)}\right) - y^{(i)}\right)^2$$

To avoid confusion, note that: $\phi\left(x^{(i)}\right) = \left[1, x^{(i)}, (x^{(i)})^2, (x^{(i)})^3\right]$

$$\mathrm{f}\left(x^{(i)}\right) = w_0 + w_1 x^{(i)} + w_2 \left(x^{(i)}\right)^2 + w_3 \left(x^{(i)}\right)^3$$





NonLinear Regression

Loss: $$\underset{w}{\operatorname{argmin}} \frac{1}{N}\sum_{n=1}^{N}\left(w^T\phi\left(x^{(i)}\right) - y^{(i)}\right)^2 = \underset{w}{\operatorname{argmin}}\|\Phi w - y\|^2$$

Where $\Phi = \left[\phi\left(x^{(1)}\right), \dots, \phi\left(x^{(N)}\right)\right]^T \in \mathbb{R}^{N\times M}$ and $w \in \mathbb{R}^M$.

Optimization:

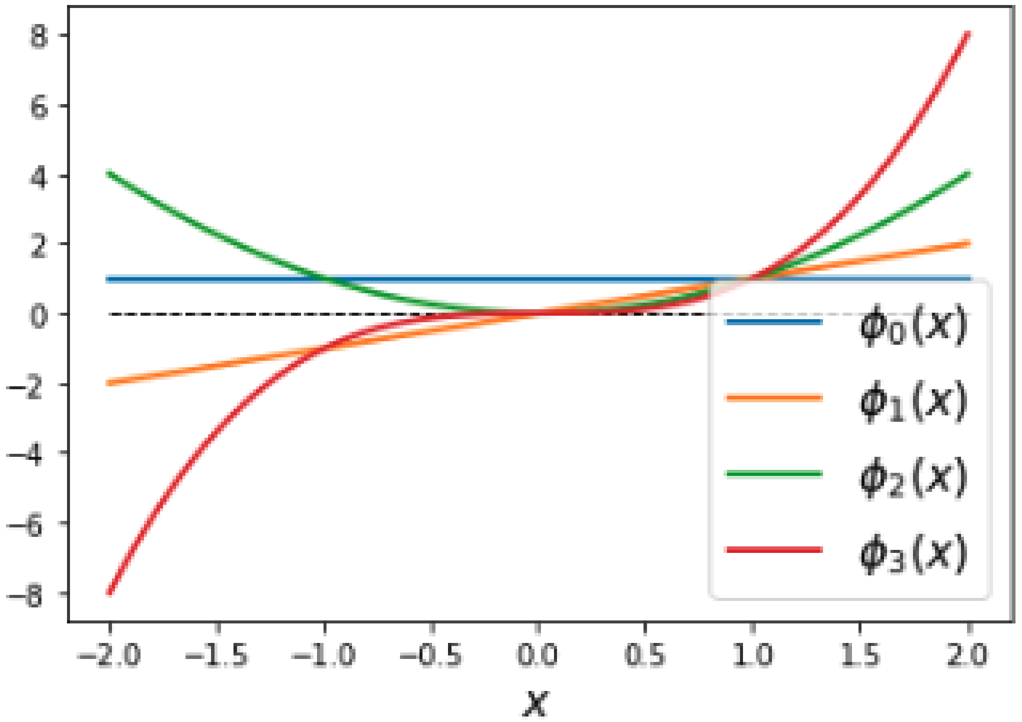
1. Closed form solution: $w^* = (\Phi^T\Phi)^{-1}\Phi^T y$
2. Gradient descent: $w^{(t)} = w^{(t-1)} - \epsilon\nabla_w Loss(w^{(t-1)})$

$$J(w) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - w^T\hat{x}^{(i)}\right)^2$$

$$W^* = (X^TX)^{-1}X^TY$$

What is the problem of Nonlinear Regression?

NonLinear Regression



The basis function is all fixed!

Can we learn the basis function?

NonLinear Regression

- Lets first look at what the learning problem might look like:

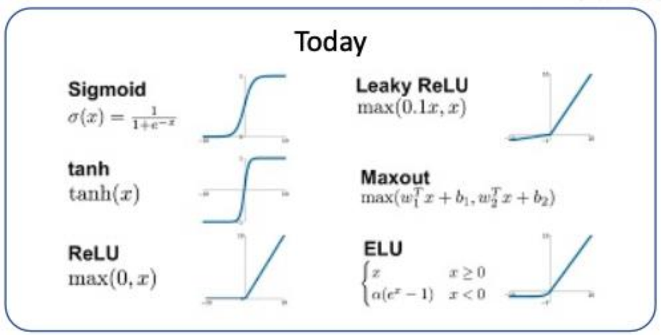
$$\underset{w}{\operatorname{argmin}} \sum_i \left(\left(\sum_j w_j \phi_j \left(x^{(i)} \right) \right) - y^{(i)} \right)^2$$

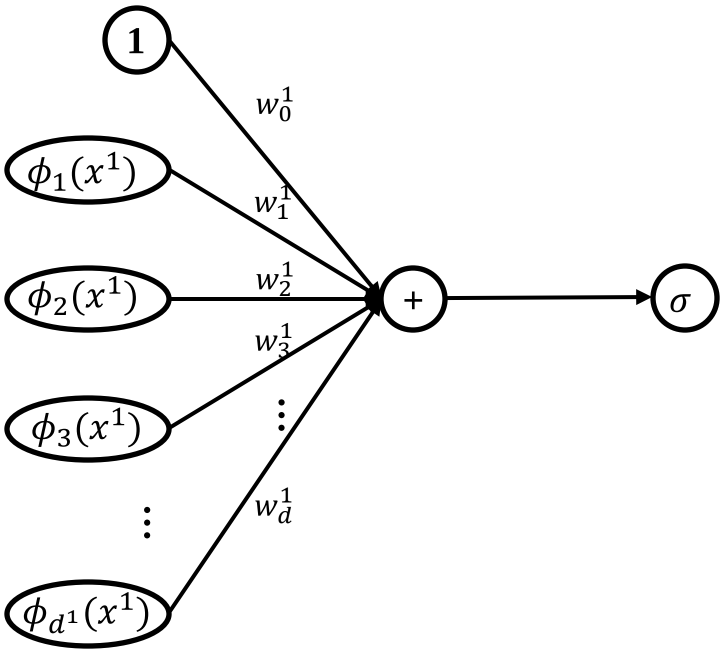
Neural Networks do this for us!

What things are learned here?
What things are fixed here?

NonLinear Regression

1-layer Multi-layer Perceptron





$$\sum_{j=0}^{d^1} w_j^1 \phi_j(x^1)$$

NonLinear Regression

- Lets first look at what the learning problem might look like:

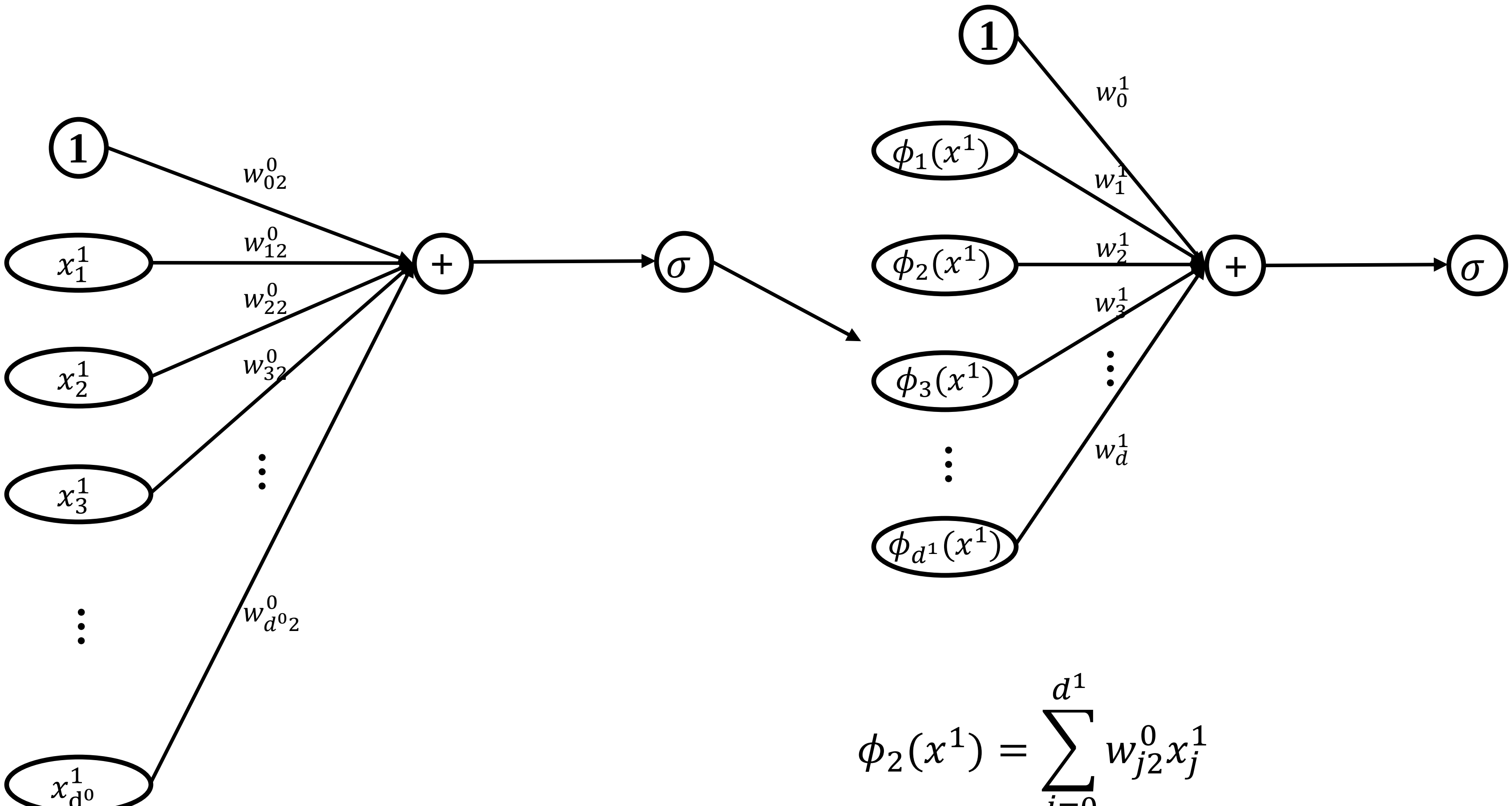
$$\underset{w, \boxed{\{\phi_j\}_{j=1}^M}}{\operatorname{argmin}} \sum_i \left(\left(\sum_j w_j \phi_j\left(x^{(i)}\right) \right) - y^{(i)} \right)^2$$

Neural Networks do this for us!

What things are learned here?
What things are fixed here?

NonLinear Regression

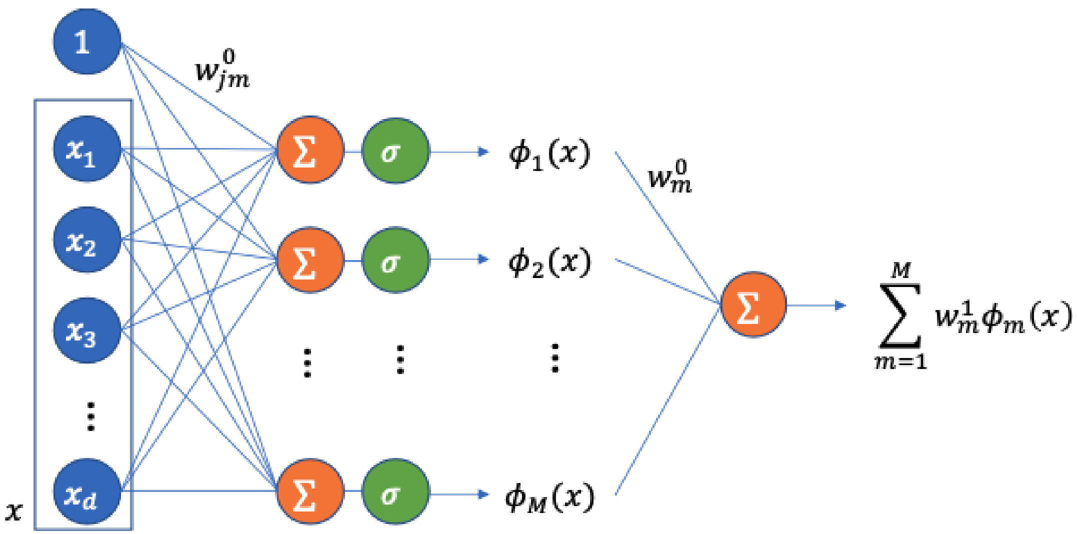
1-hidden layer Multi-layer Perceptron



$$\phi_2(x^1) = \sum_{j=0}^{d^1} w_{j2}^0 x_j^1$$

NonLinear Regression

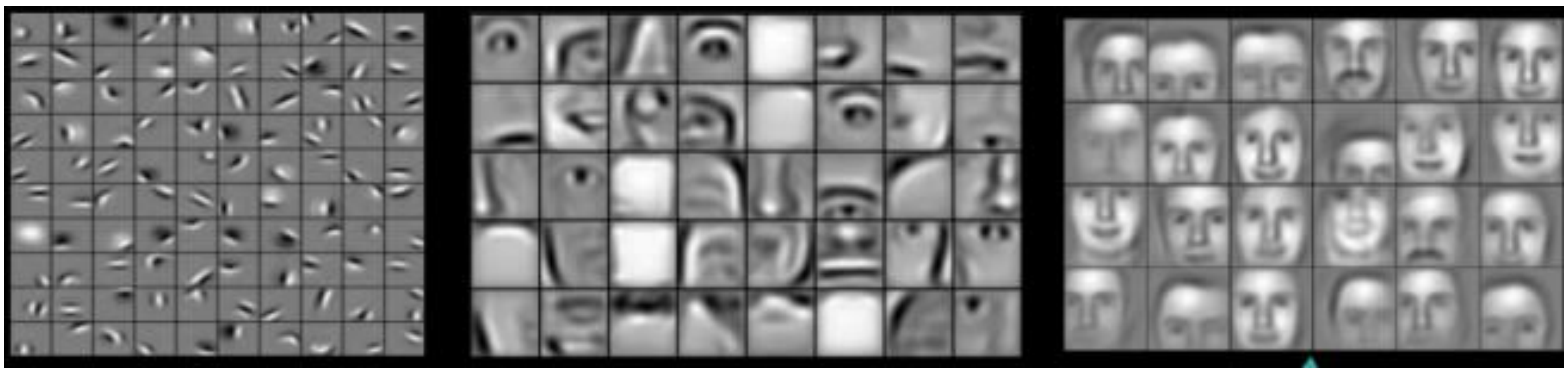
1-hidden layer Multi-layer Perceptron



$$f(x) = \sum_{m=1}^{M} w^1_m \sigma\left(\sum_{j=1}^{d} W^0_{jm}\, x_j\right)$$

Example

- **Activations at hidden layers can be viewed as features extracted as functions of inputs**
- **Every hidden layer represents a level of abstraction**
  - ***Complex features are compositions of simpler features***

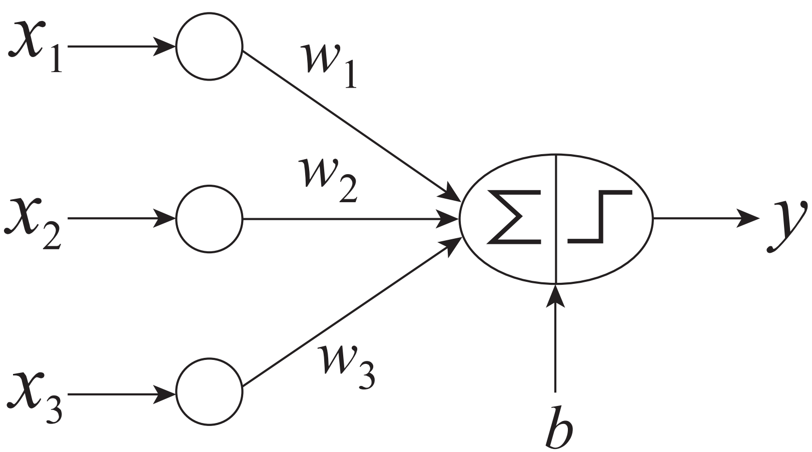


- **Number of layers is known as depth of ANN**
  - ***Deeper networks express complex hierarchy of features***

Question?

1. "Judge a man by his questions rather than by his answers."
   – Voltaire
2. "If I had an hour to solve a problem, I'd spend 55 minutes thinking about the problem and 5 minutes thinking about solutions."
   – Albert Einstein
3. "The art and science of asking questions is the source of all knowledge."
   – Thomas Berger
4. "Asking the right questions takes as much skill as giving the right answers."
   – Robert Half
5. "The wise man doesn't give the right answers, he poses the right questions."
   – Claude Lévi-Strauss
6. "Great questions make great companies."
   – Peter Drucker

Linear Regression



$$\sigma(w^{\mathrm{T}}x + b)$$

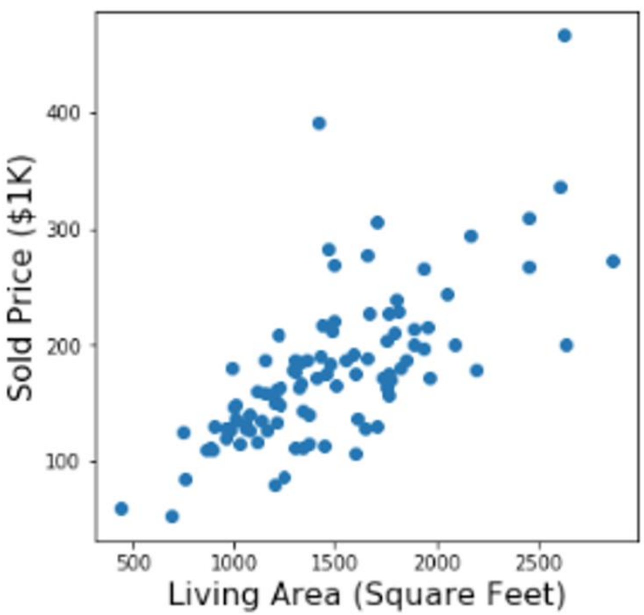
$$\underset{w}{\operatorname{argmin}} \boxed{\frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - w^T\hat{x}^{(i)}\right)^2} = \underset{w}{\operatorname{argmin}} \boxed{\frac{1}{N}\|y - Xw\|^2}$$

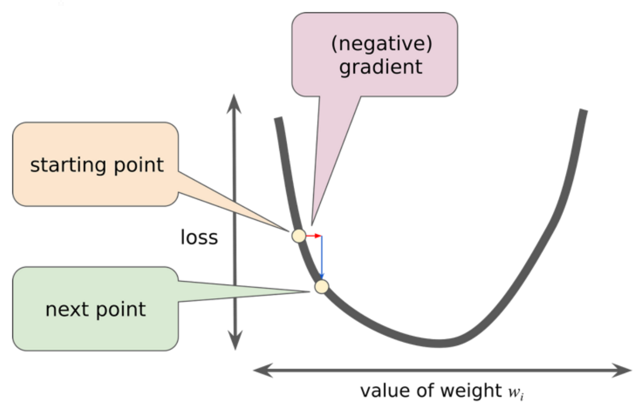
Loss/Cost Function

Analytical Solution

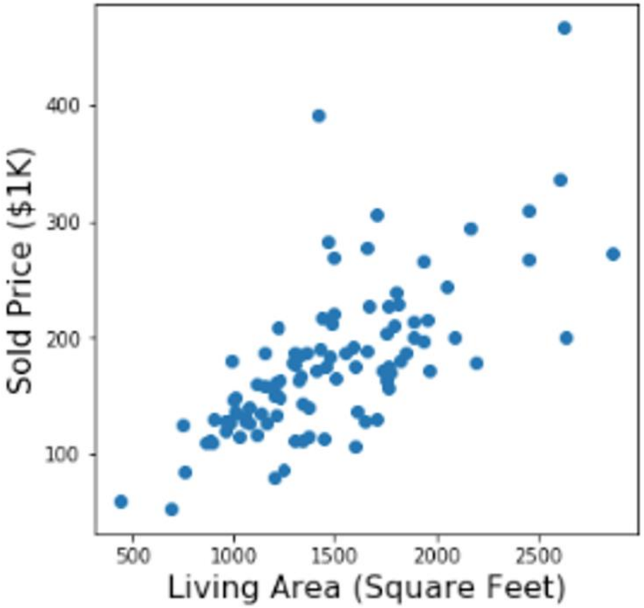
Gradient Descent

$$\nabla J(W) = -\frac{2}{N}X^TY + \frac{2}{N}X^TXW \qquad W^* = (X^TX)^{-1}X^TY$$





Linear Regression



$$y = \sigma(w^{\mathrm{T}}x + b)$$

$$y = \sigma(w^{\mathrm{T}}\phi(x) + b)$$

$$\nabla J(W) = -\frac{2}{N}X^T Y + \frac{2}{N}X^T X W$$

$$\nabla J(W) = -\frac{2}{N}\phi(X)^{\mathrm{T}}Y + \frac{2}{N}\phi(X)^T\phi(X)W$$

$$W^* = (X^T X)^{-1} X^T Y$$

$$W^* = (\phi(X)^T\phi(X))^{-1}\phi(X)^T Y$$

Linear Regression

$$J(w) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - w^T\hat{x}^{(i)}\right)^2$$

$$\nabla J(w) = \frac{\partial J(w)}{\partial w}$$

$$J(w) = \frac{1}{N}\sum_{i=1}^{N}(y^{(i)} - w^T\hat{x}^{(i)})^2$$

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$$w_0 := w_0 + \frac{2\alpha}{N}\sum_{i=1}^{N}(y^{(i)} - (w_0 + w_1x_1^{(i)}))$$

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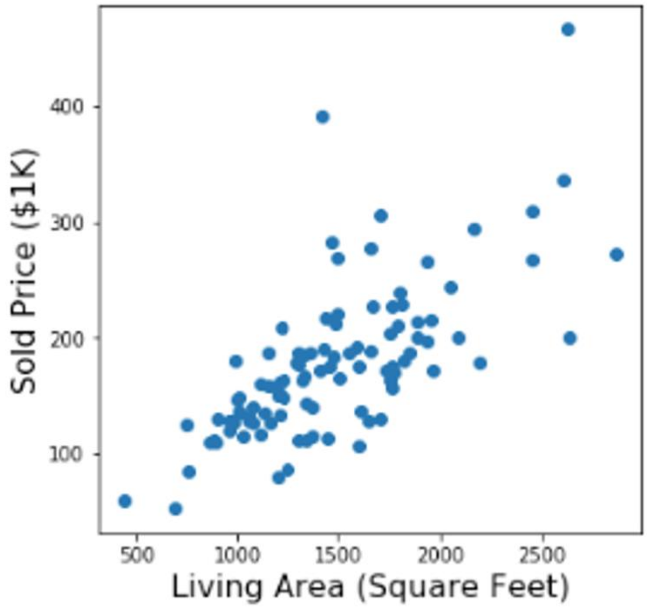
Linear Regression

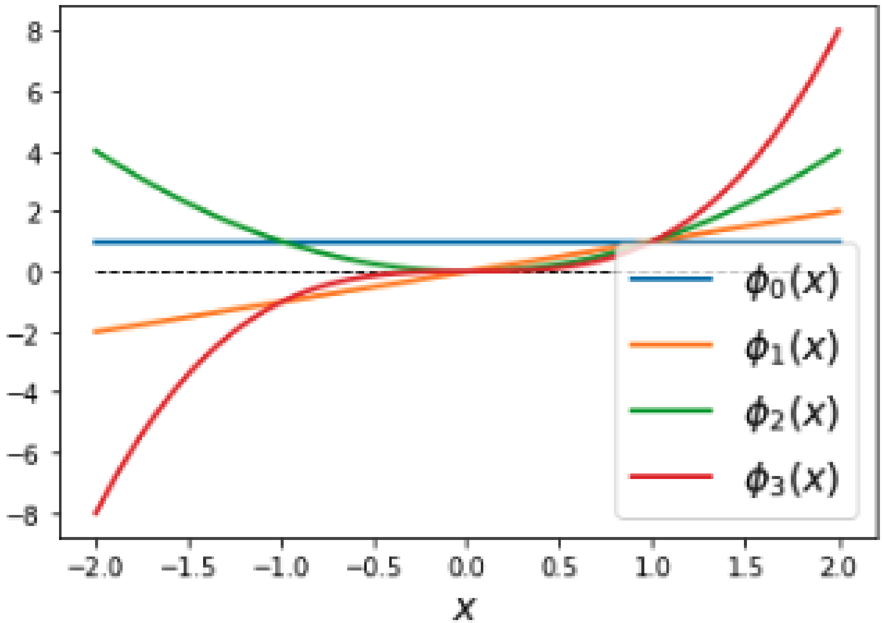


$$y = w_1 x + w_0$$

$$w_0 := w_0 + \frac{2\alpha}{N}\sum_{i=1}^{N}(y^{(i)} - (w_0 + w_1 x_1^{(i)}))$$

$$w_1 := w_1 + \frac{2\alpha}{N}\sum_{i=1}^{N}(y^{(i)} - (w_0 + w_1 x_1^{(i)}))x_1^{(i)}$$

Non-Linear Regression



$$y = \sigma(w^{\mathrm{T}}x + b)$$

$$y = \sigma(w^{\mathrm{T}}\phi(x) + b)$$

$$\nabla J(W) = -\frac{2}{N}X^TY + \frac{2}{N}X^TXW$$

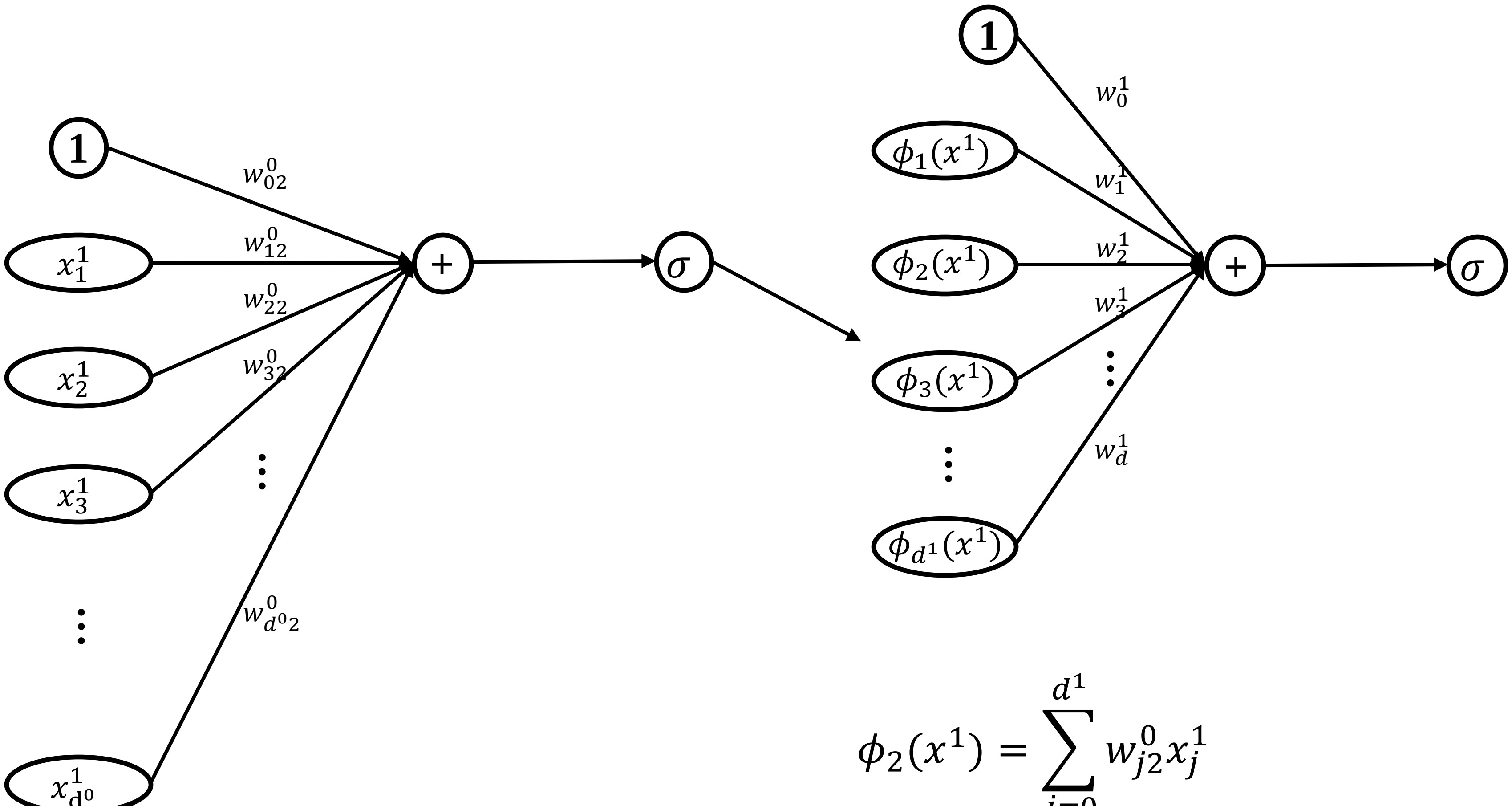
$$\nabla J(W) = -\frac{2}{N}\phi(X)^{\mathrm{T}}Y + \frac{2}{N}\phi(X)^T\phi(X)W$$

$$W^* = (X^TX)^{-1}X^TY$$

$$W^* = (\phi(X)^T\phi(X))^{-1}\phi(X)^TY$$

Multi-NonLinear Regression

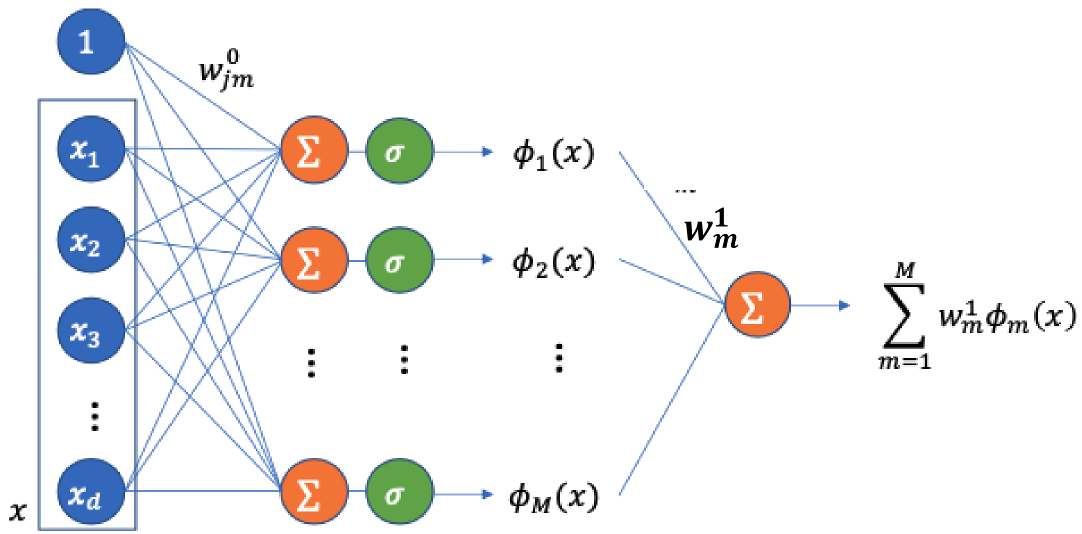
1-hidden layer Multi-layer Perceptron



$$\phi_2(x^1) = \sum_{j=0}^{d^1} w_{j2}^0 x_j^1$$

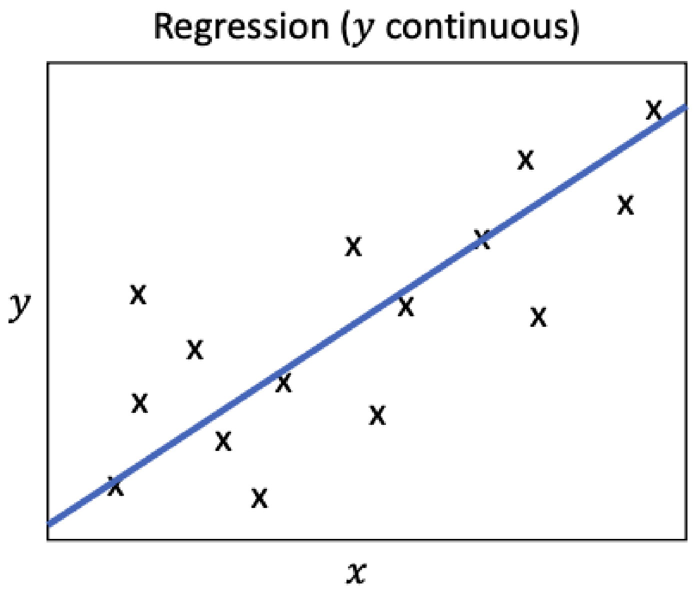
Multi-NonLinear Regression

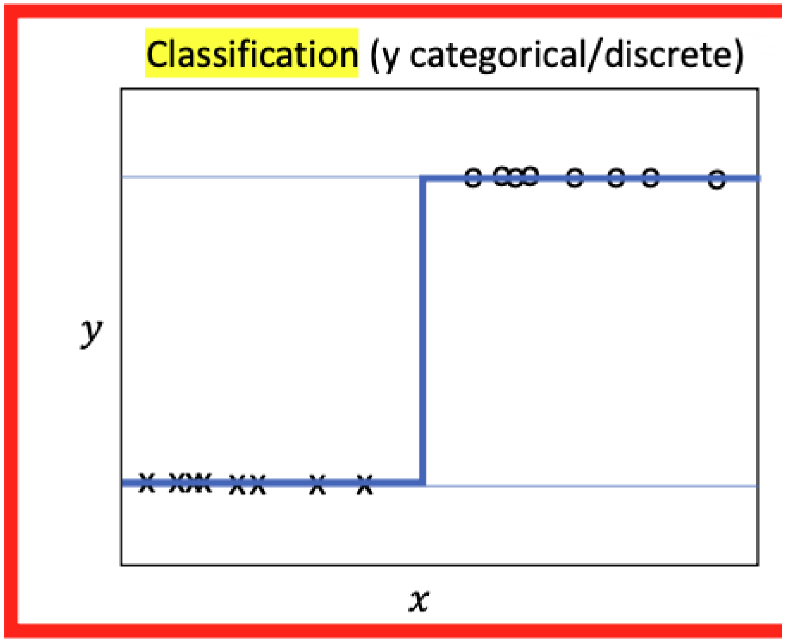
1-hidden layer Multi-layer Perceptron



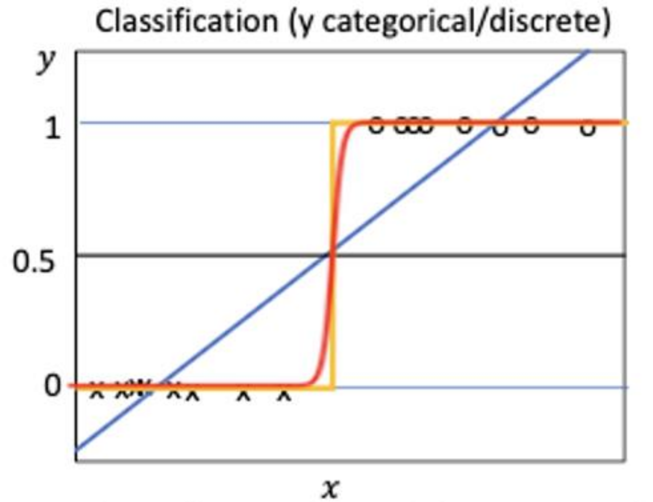
$$f(x) = \sum_{m=1}^{M} w_m^1 \sigma\left(\sum_{j=1}^{d} W_{jm}^0 x_j\right)$$

Classification





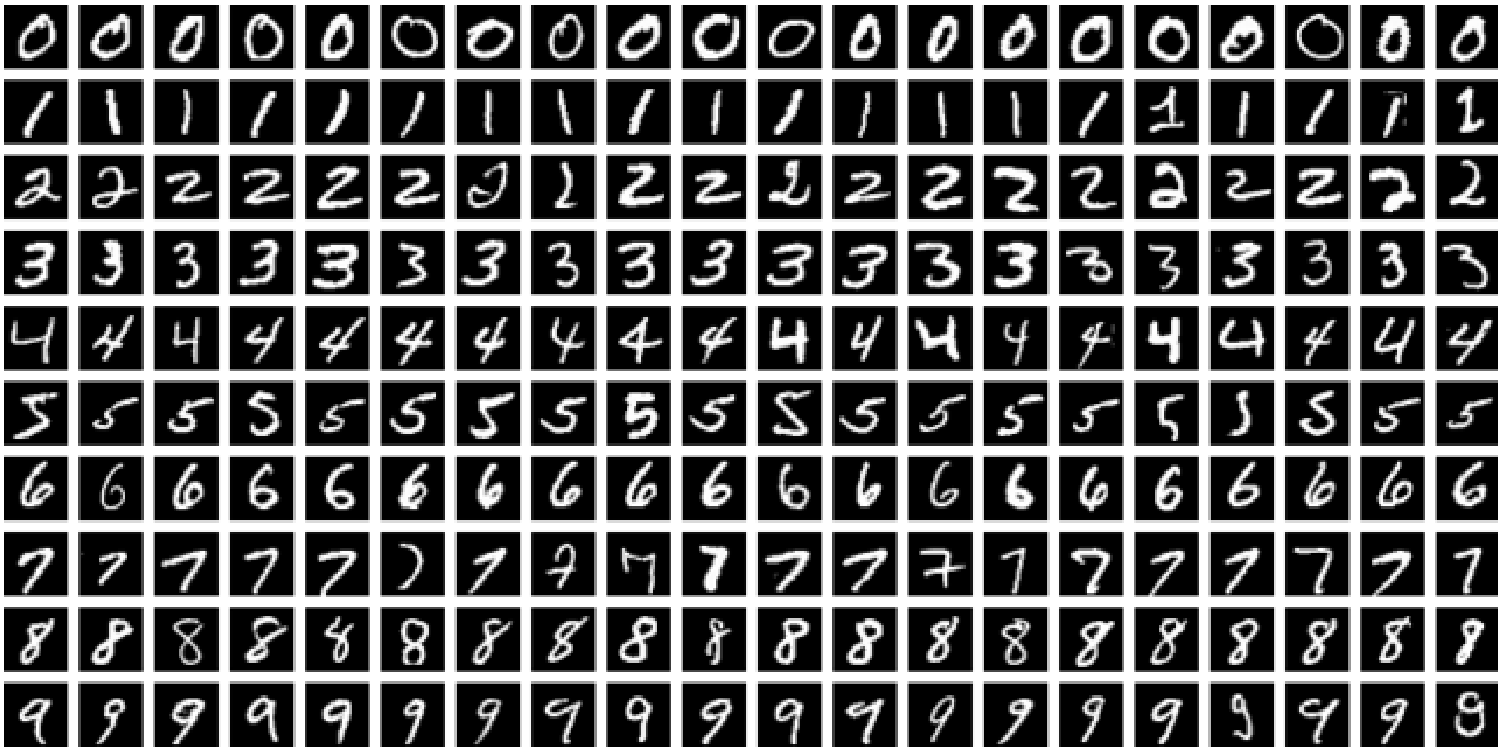
Classification



What loss should we use?

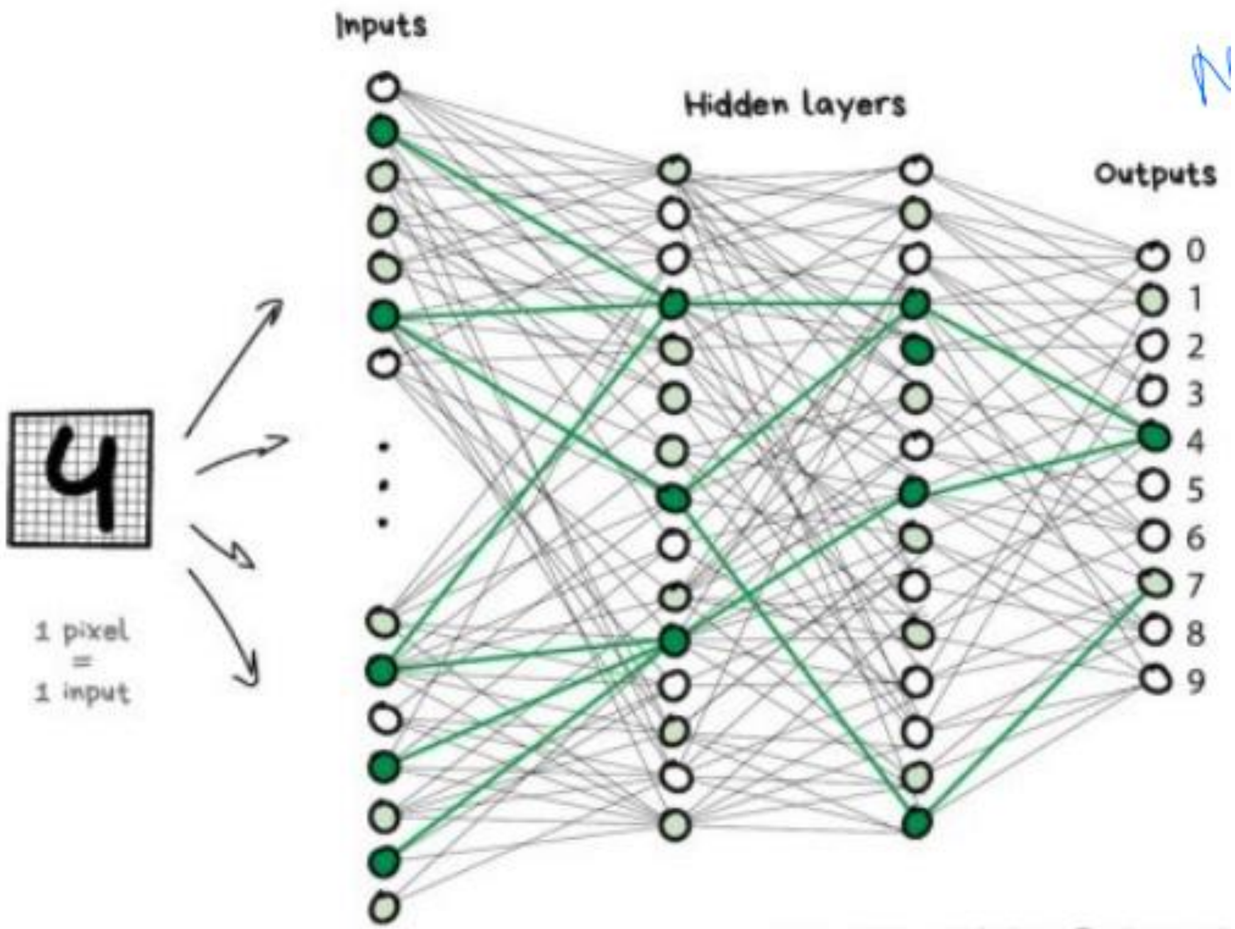
$$\mathcal{L}(w) = -\sum_{i=1}^{N} y^{(i)} \log\left(f\left(x^{(i)}\right)\right) + \left(1 - y^{(i)}\right) \log(1 - f(x_i))$$

MINIST Dataset



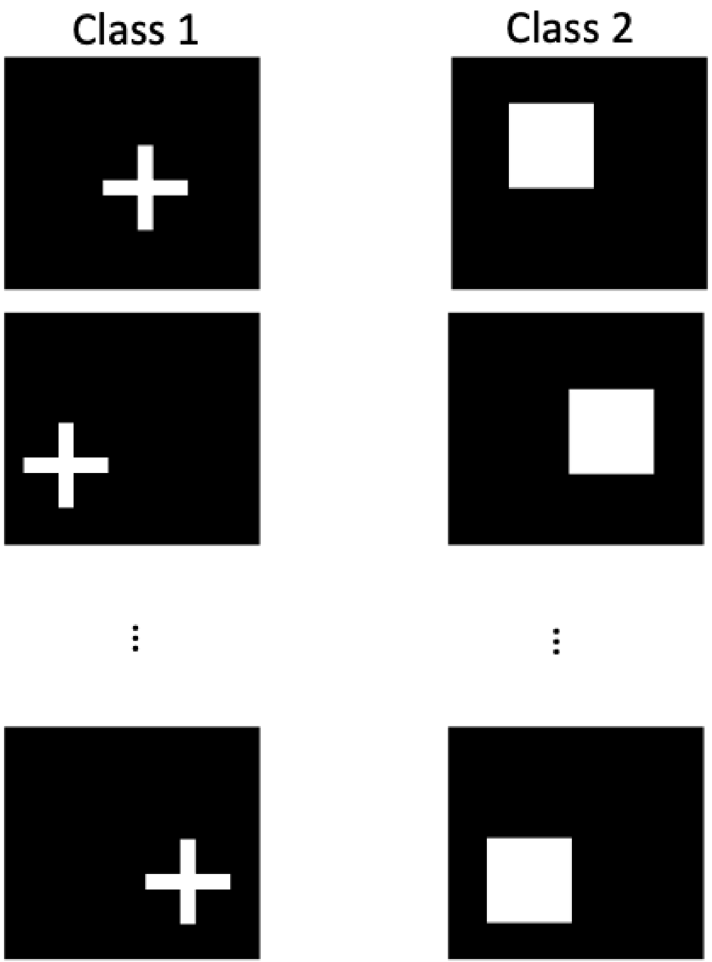
A 256x256 (RGB) image $\Longrightarrow$ ~200K dimensional input x

MLP for MINIST



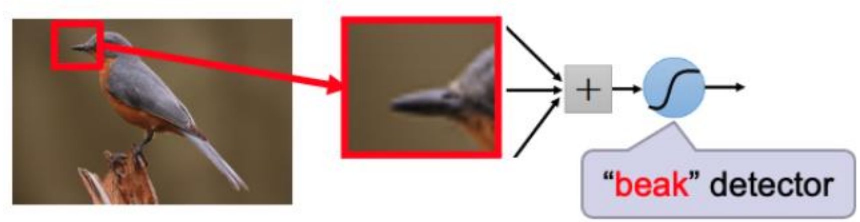
A fully connected network would need a very large number of parameters, very likely to overfit the data

CNN



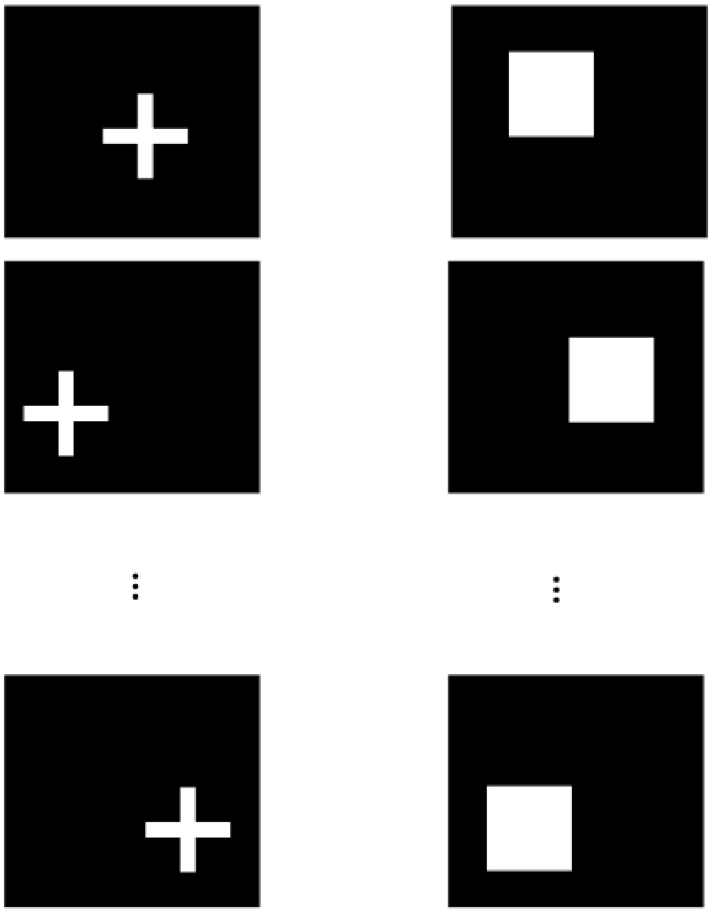
- The features of these classes are spatially local.
- Translation does not change the identity of the classes, i.e., we require a translation equivariant model.
- MLP is not a good match to this problem

Can represent a small region with fewer parameters



CNN

Class 1 Class 2



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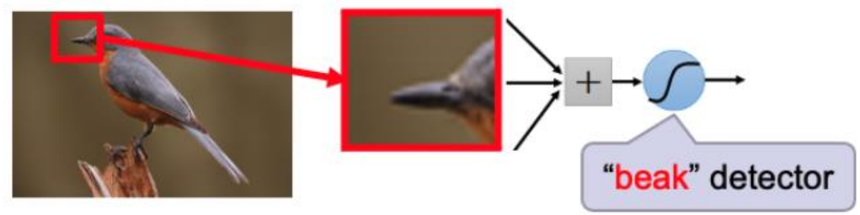
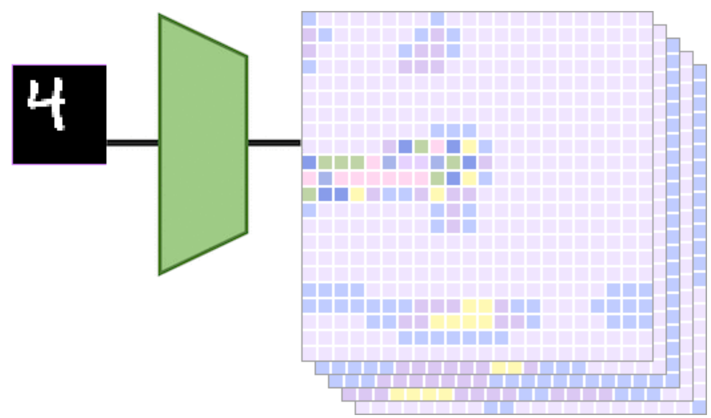
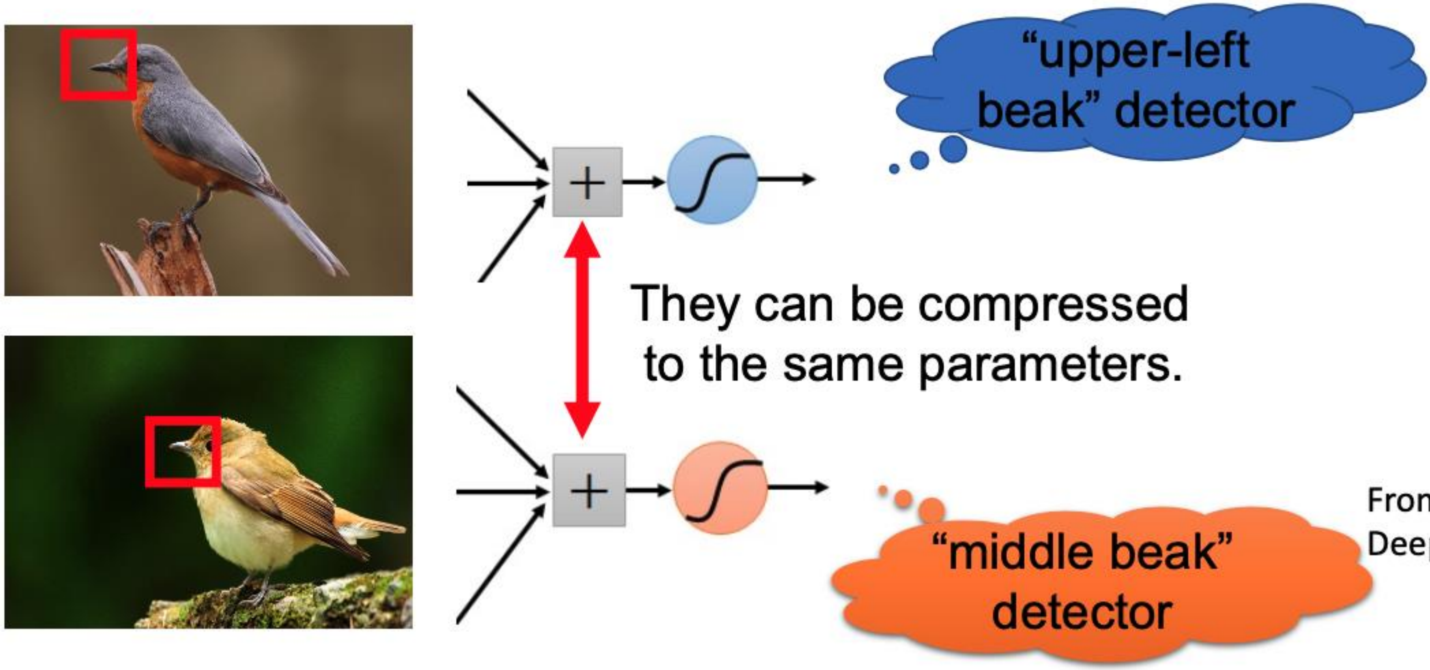




CNN

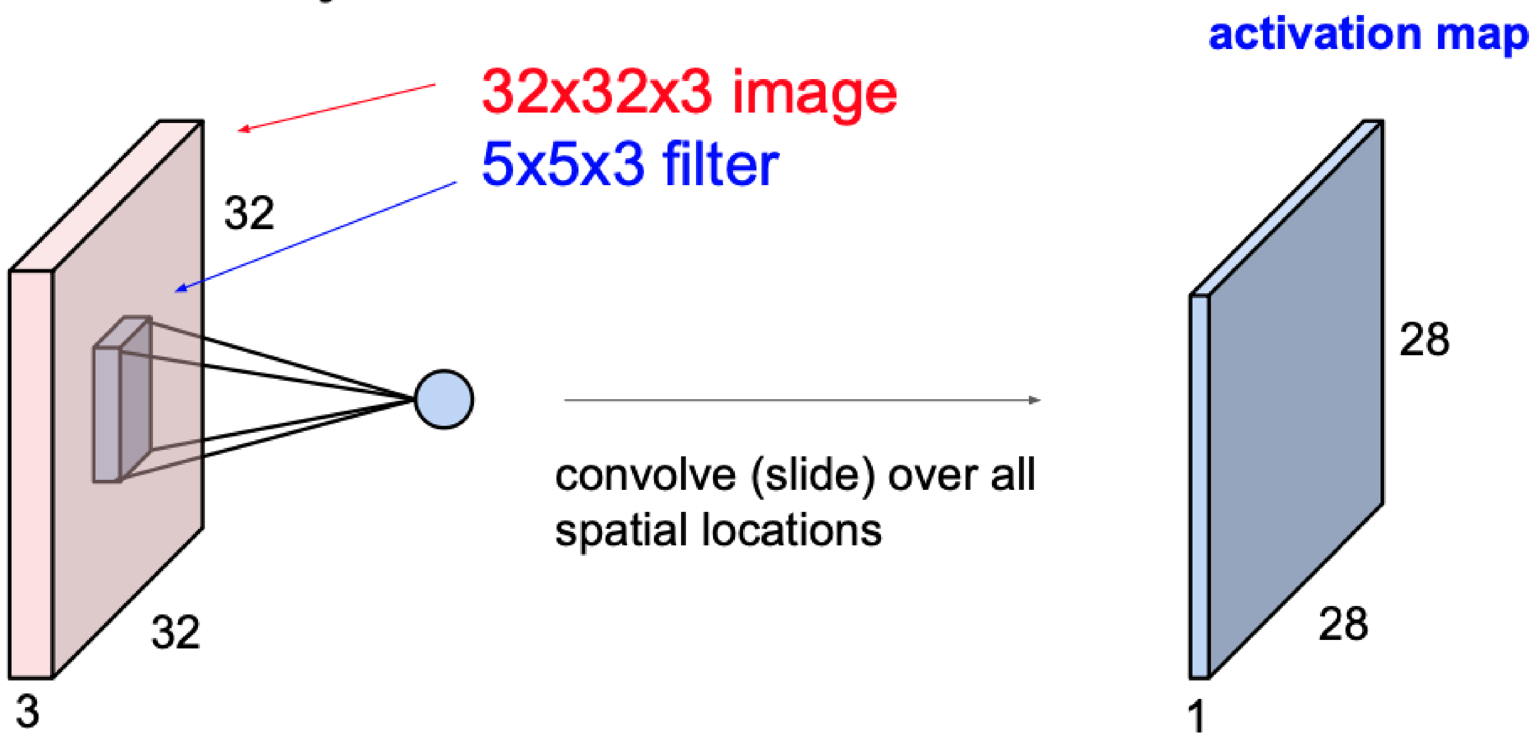


From U-Waterloo's
Deep Learning Course

What about training a lot of such "small" detectors and each detector must "move around".

CNN

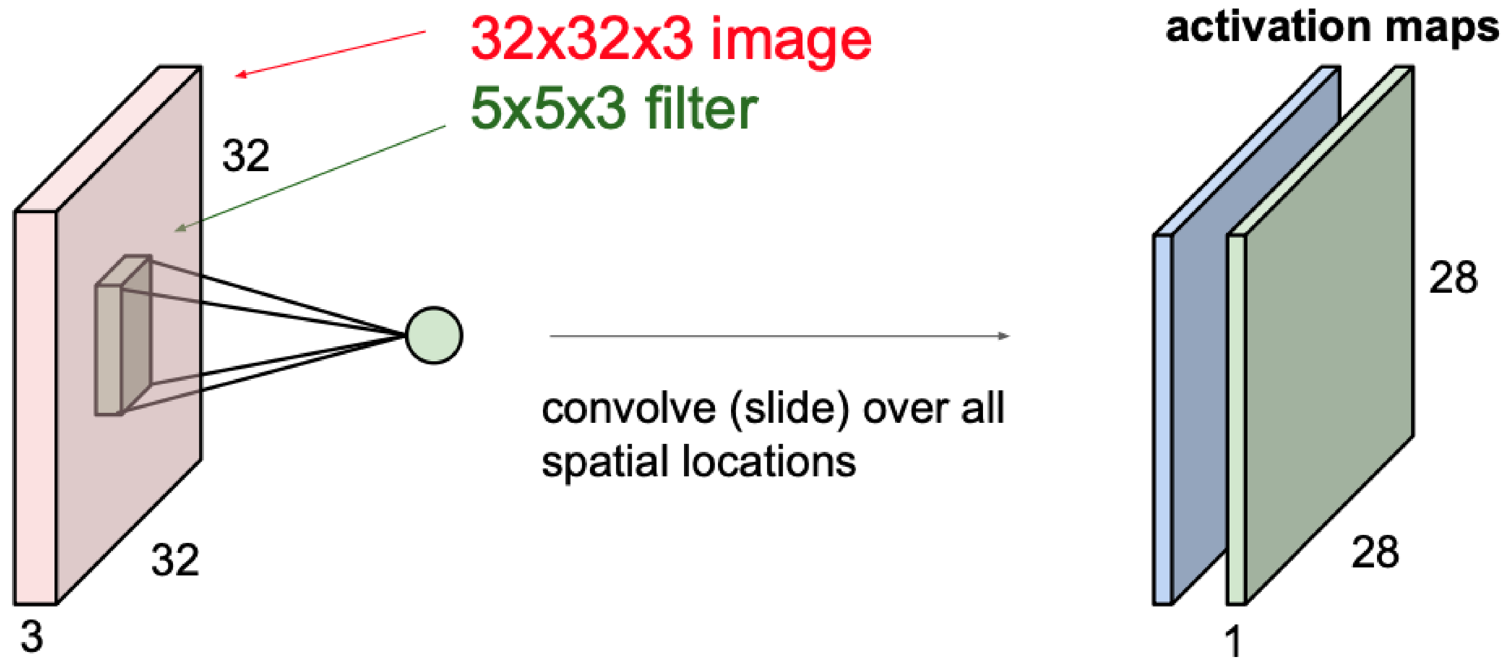
Convolution Layer



CNN

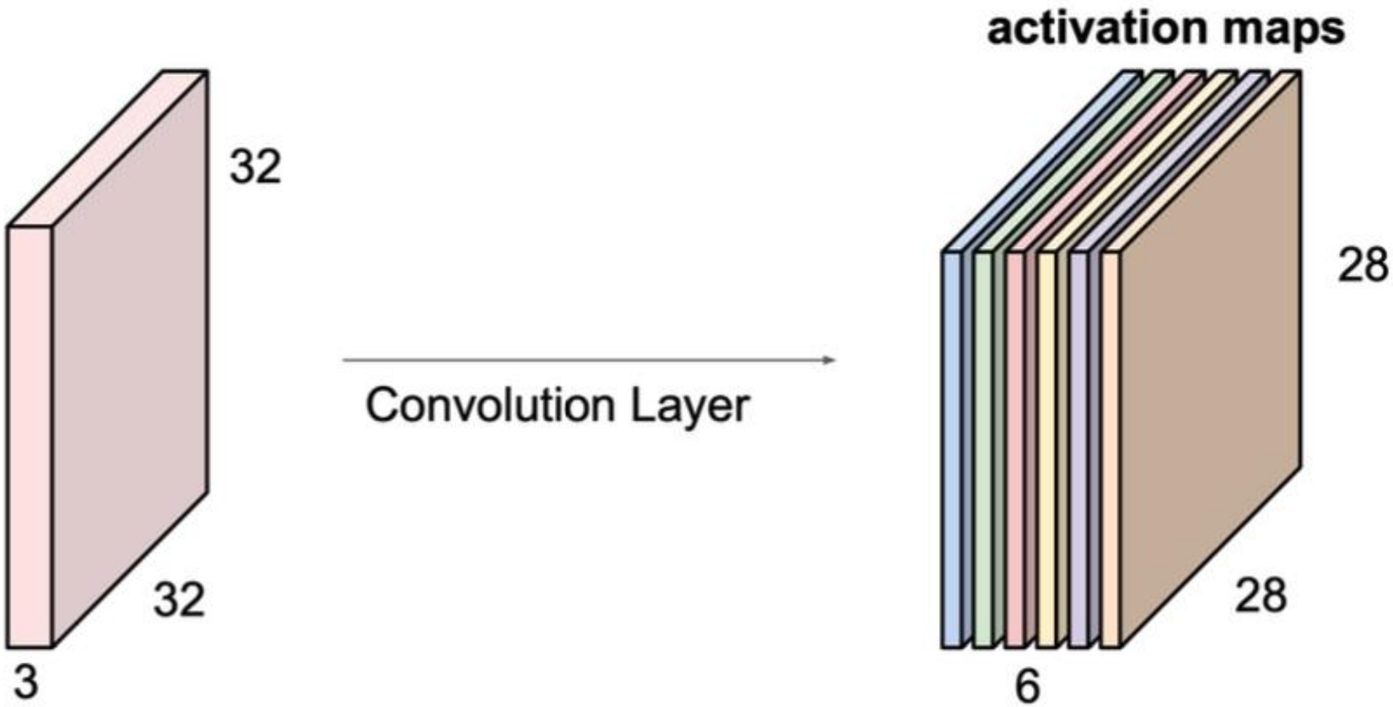
Convolution Layer

consider a second, green filter



CNN

For example, if we had 6 5x5 filters, we'll get 6 separate activation maps:



We stack these up to get a "new image" of size 28x28x6!

CNN

1	0	0	0	0	1
0	1	0	0	1	0
0	0	1	1	0	0
1	0	0	0	1	0
0	1	0	0	1	0
0	0	1	0	1	0

6 x 6 image

1	-1	-1
-1	1	-1
-1	-1	1

Filter 1

-1	1	-1
-1	1	-1
-1	1	-1

Filter 2

⋮ ⋮

Each filter detects a small pattern (3 x 3).

CNN

stride=1

1	0	0	0	0	1
0	1	0	0	1	0
0	0	1	1	0	0
1	0	0	0	1	0
0	1	0	0	1	0
0	0	1	0	1	0

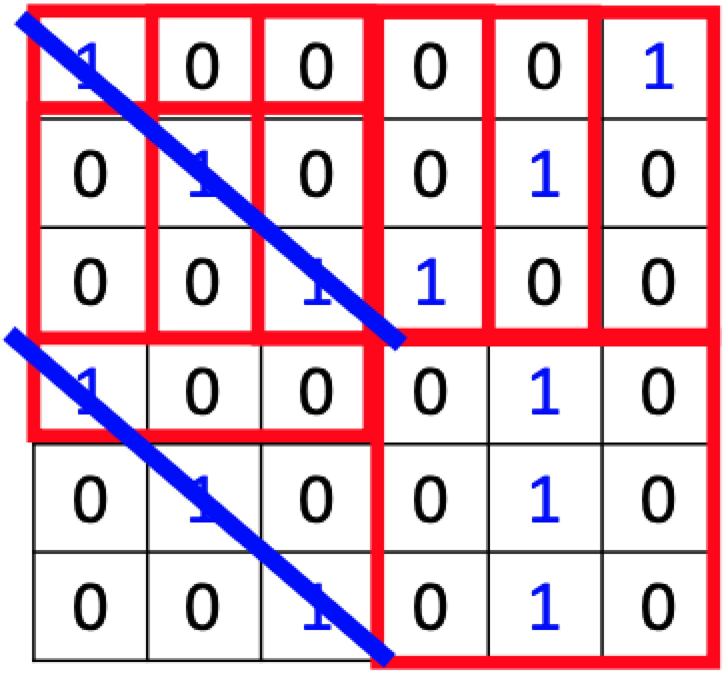
6 x 6 image

Dot product $\rightarrow$ 3 -1

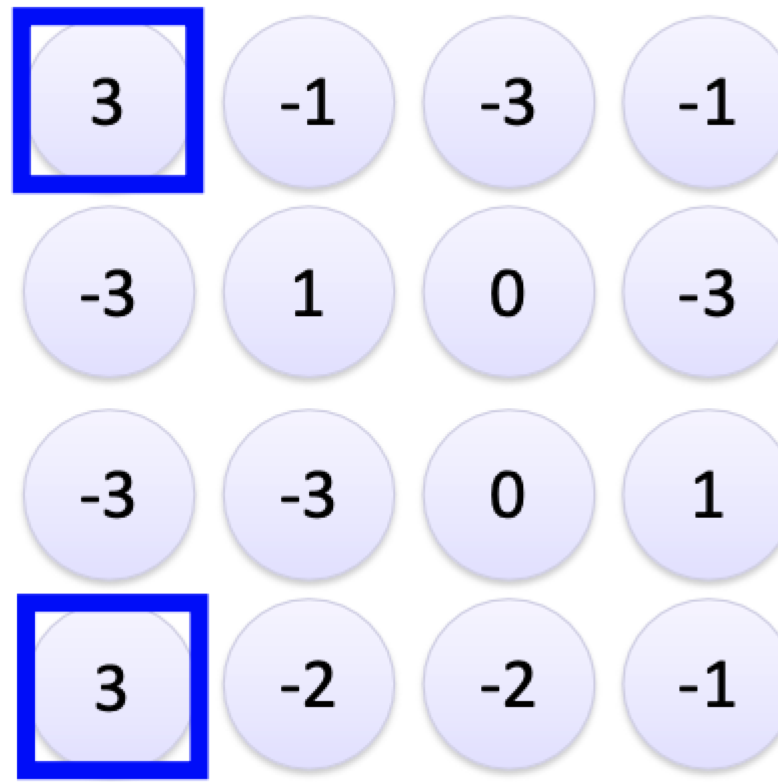
1	-1	-1
-1	1	-1
-1	-1	1

Filter 1

CNN



6 x 6 image



CNN

Convolutions (typically with *prespecified* filters) are a common operation in many computer vision applications

Original image z

Gaussian blur

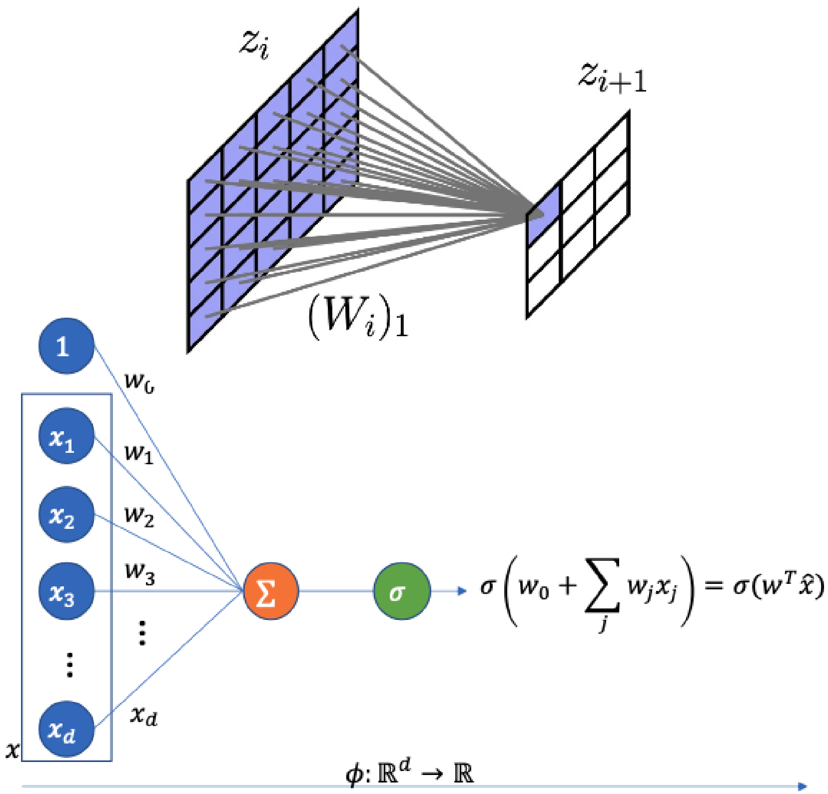
Image gradient

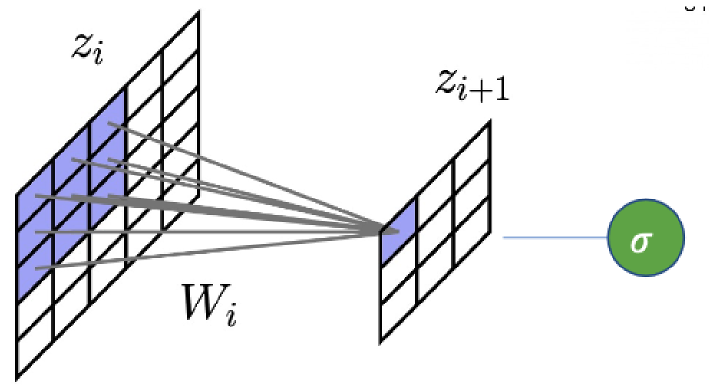
$$z * \begin{bmatrix} 1 & 4 & 7 & 4 & 1 \\ 4 & 16 & 26 & 16 & 4 \\ 7 & 26 & 41 & 26 & 7 \\ 4 & 16 & 26 & 16 & 4 \\ 1 & 4 & 4 & 4 & 1 \end{bmatrix} /273$$

$$\left(\left(z * \begin{bmatrix} -1 & 0 & 1 \\ -2 & 0 & 2 \\ -1 & 0 & 1 \end{bmatrix} \right)^2 + \left(z * \begin{bmatrix} -1 & -2 & -1 \\ 0 & 0 & 0 \\ 1 & 2 & 1 \end{bmatrix} \right)^2 \right)^{\frac{1}{2}}$$

7

CNN





Convolution is a linear operator

We need to follow convolution with a nonlinearity (e.g., ReLU) to get nonlinear functions.

CNN

bird

bird

1	-1	-1
-1	1	-1
-1	-1	1

Filter 1

-1	1	-1
-1	1	-1
-1	1	-1

Filter 2

3 ⇐

3	-1	-3	-1
-3	1	0	-3
-3	-3	0	1
3	-2	-2	-1

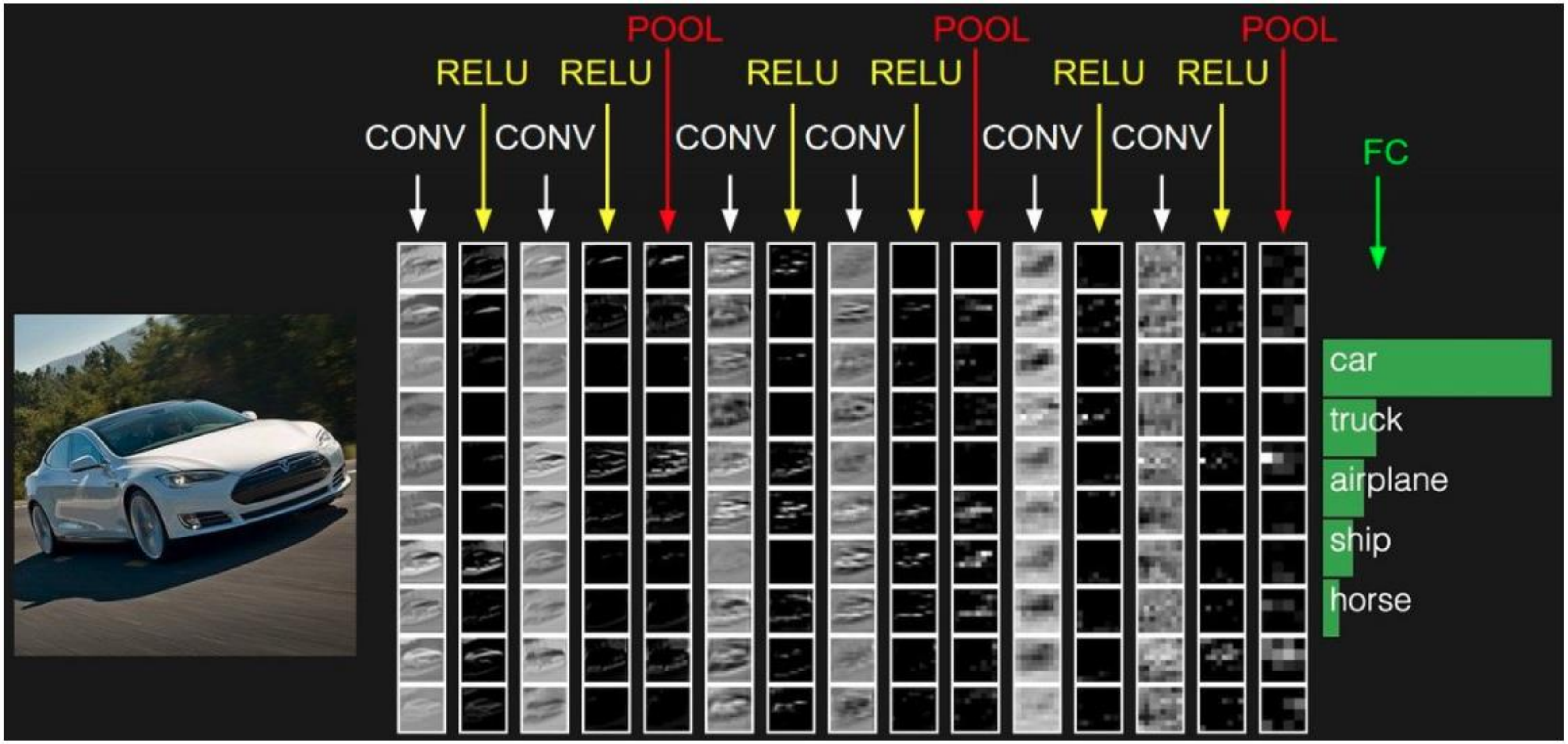
⇒ 0

3 ⇐

⇒ 1

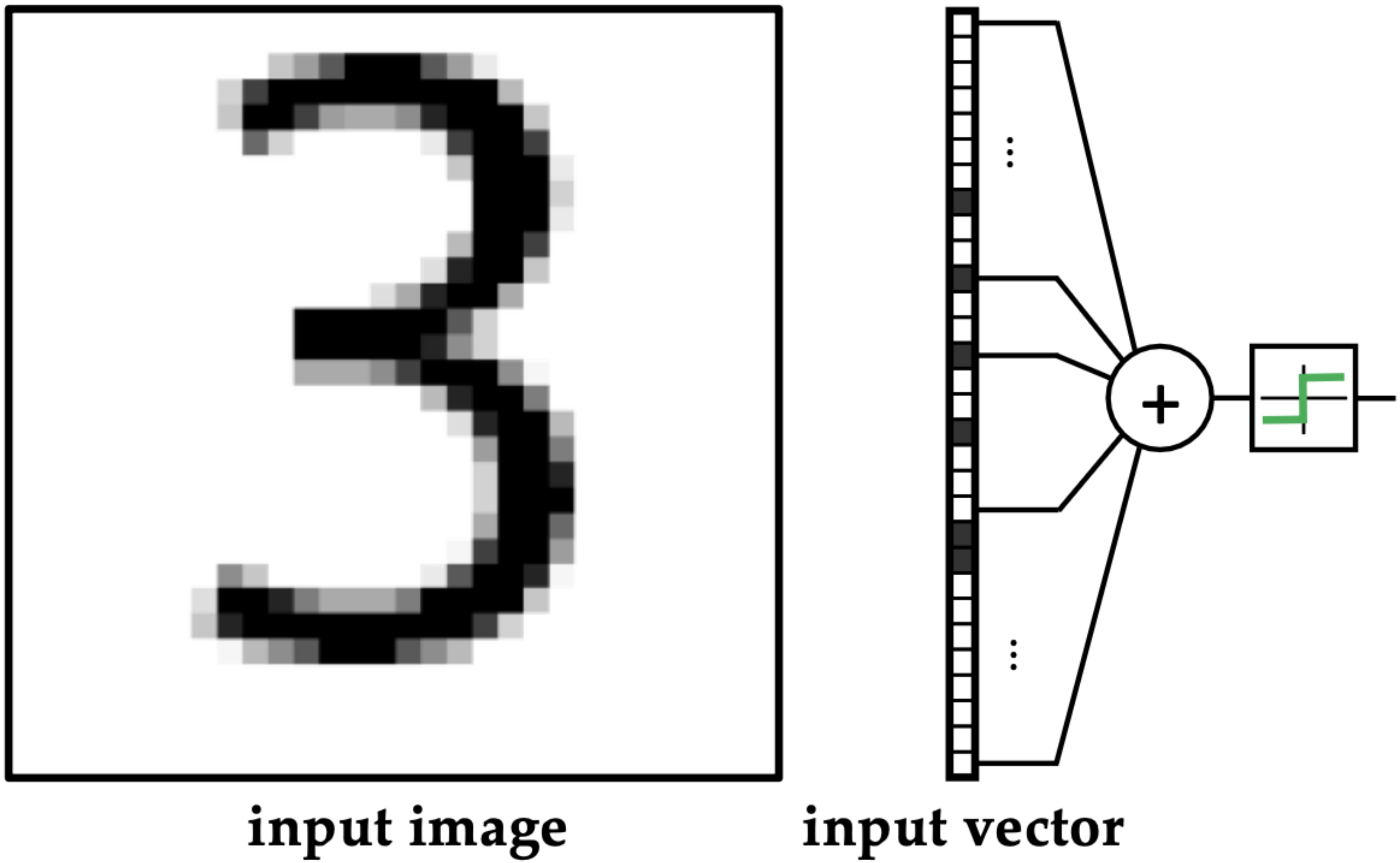
-1	-1	-1	-1
-1	-1	-2	1
-1	-1	-2	1
-1	0	-4	3

CNN

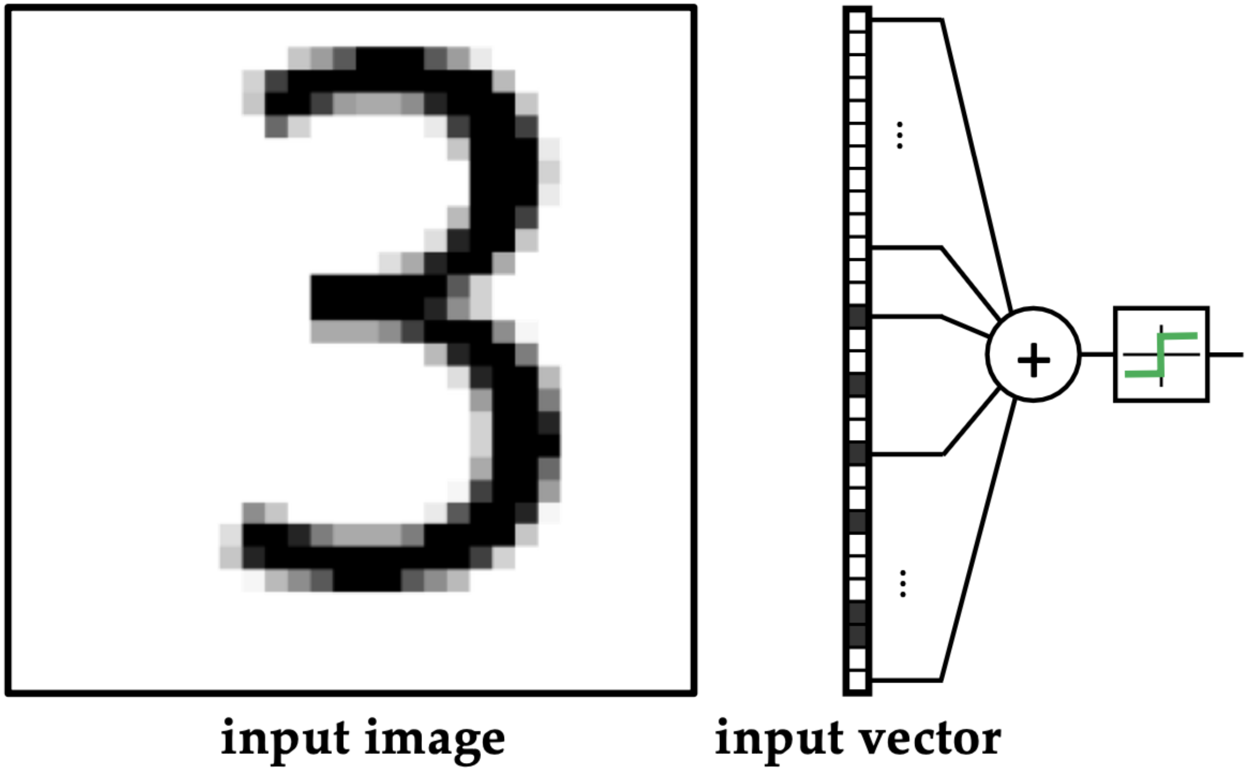


POOL
POOL
POOL
RELU
RELU
RELU
RELU
RELU
RELU
CONV
CONV
CONV
CONV
CONV
CONV
FC
car
truck
airplane
ship
horse

Equivariant and Invariant



Equivariant and Invariant

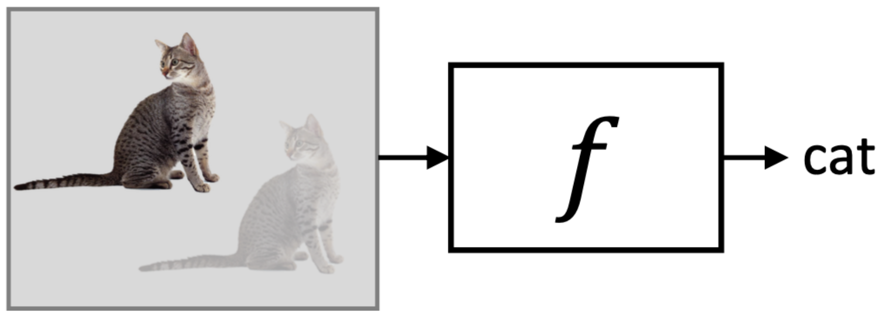


must learn shift invariance from data!

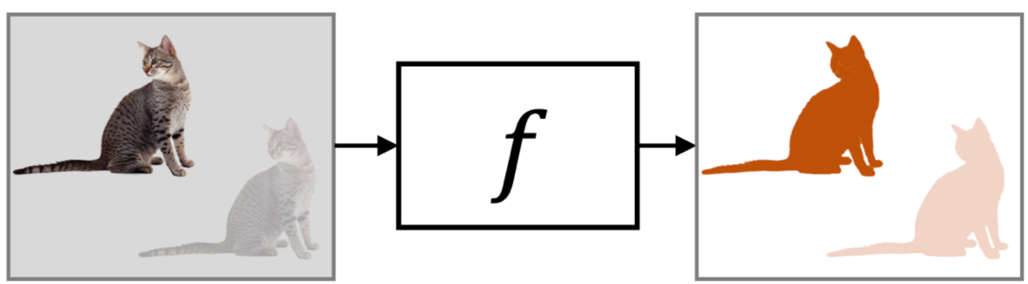
Code Demo

Equivariant and Invariant

$\mathfrak{G}$-invariance $\quad f(\rho(\mathfrak{g})x) = f(x)$



$\mathfrak{G}$-equivariance $\quad f(\rho(\mathfrak{g})x) = \rho(\mathfrak{g})f(x)$



Equivariant and Invariant

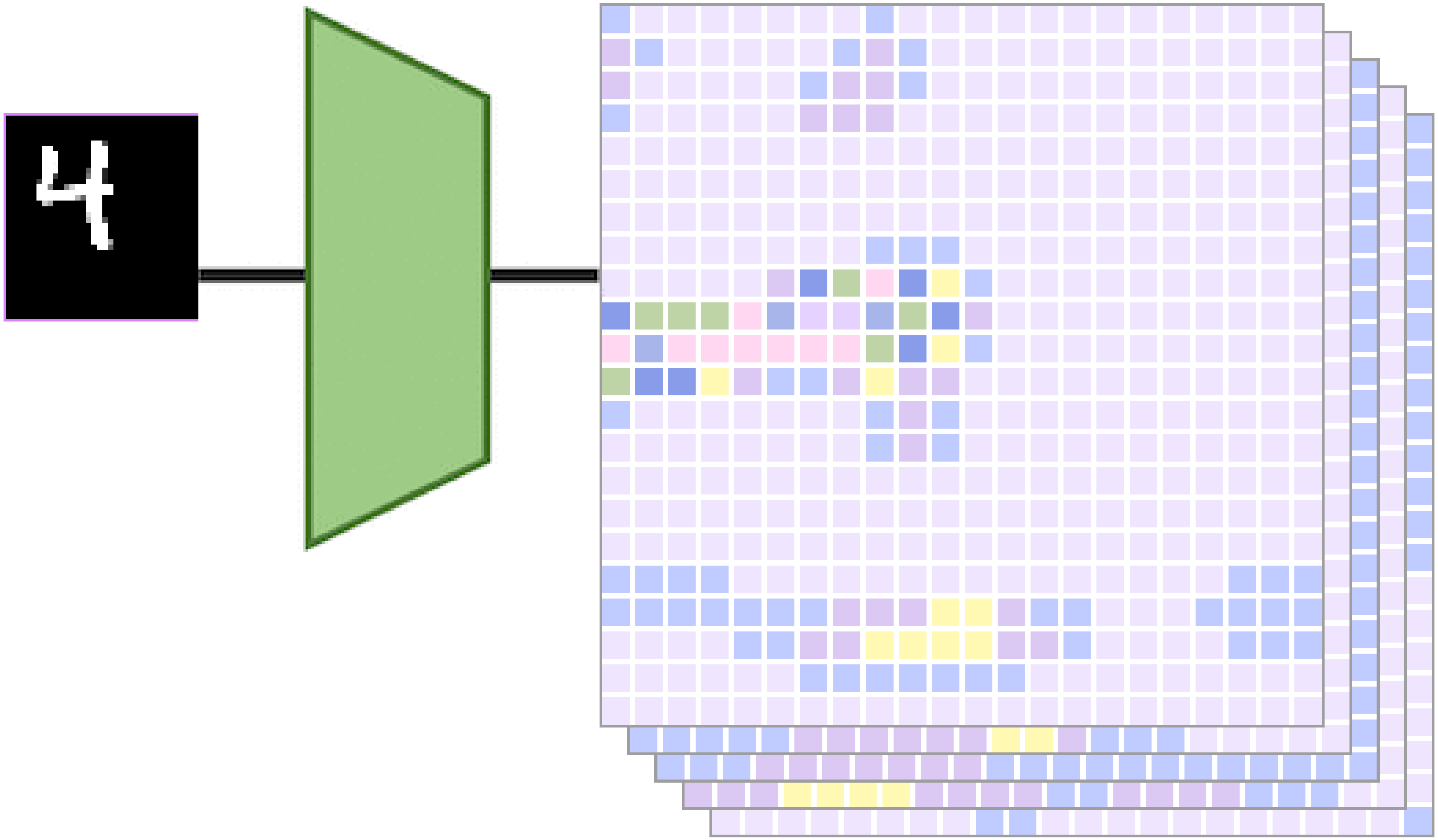
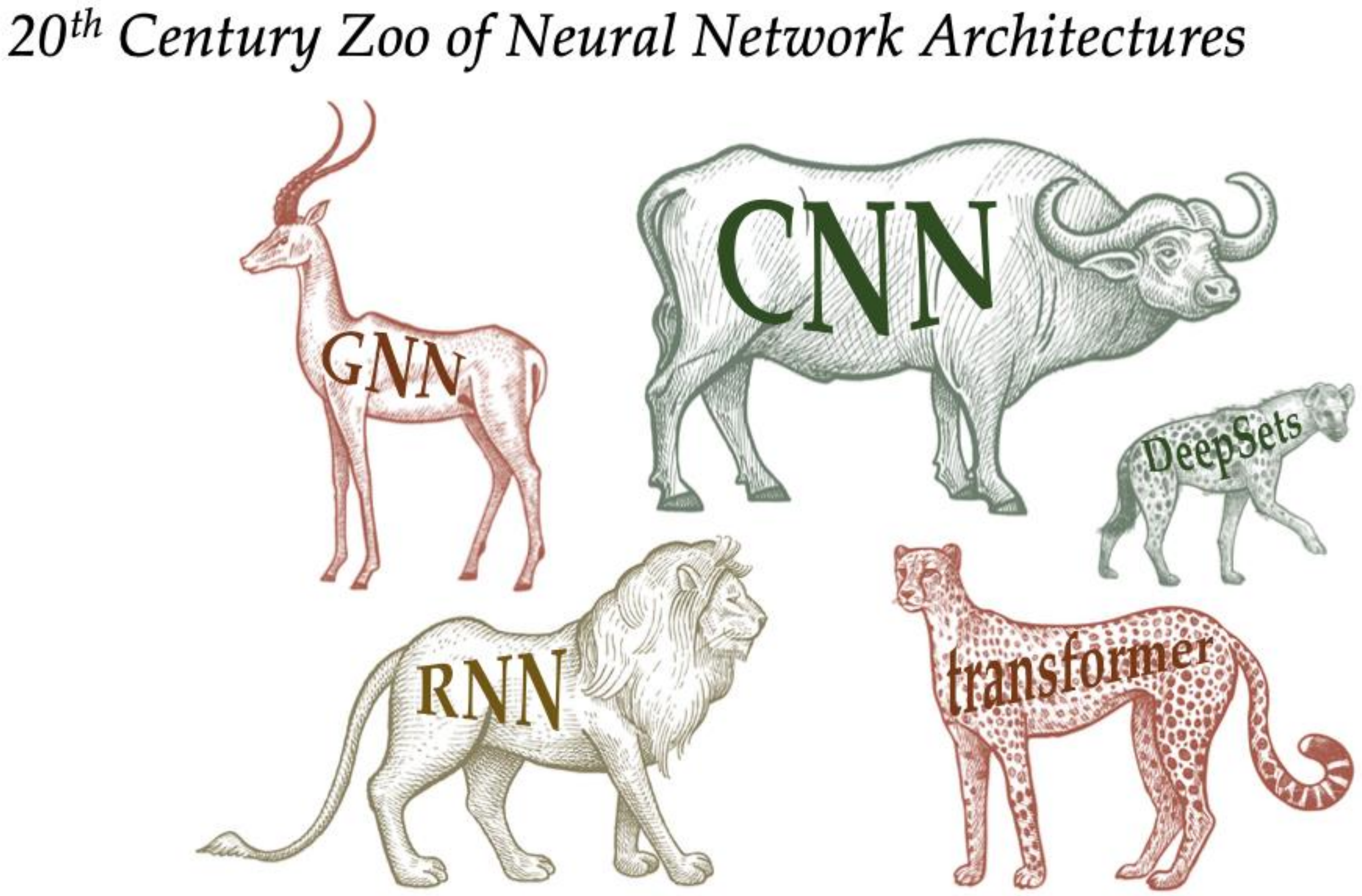


Image Convolution is ?

DNNs

Deep Neural Networks

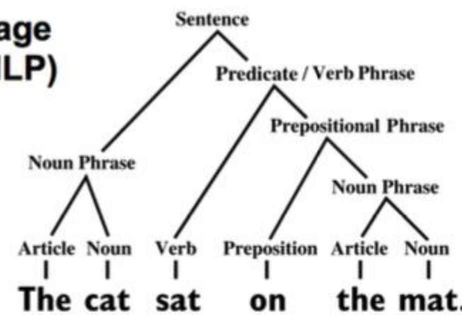


DNNs

IMAGENET

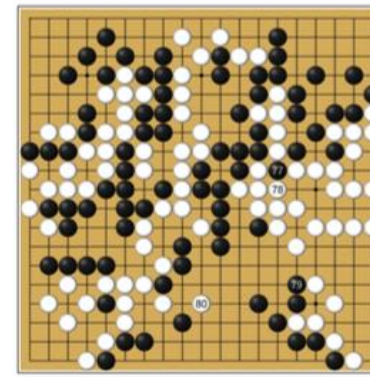
Speech data

Natural language processing (NLP)



...

Grid games



Deep neural nets that exploit:

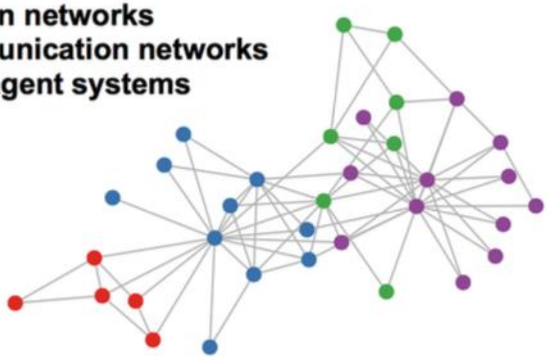
- translation equivariance (weight sharing)
- hierarchical compositionality

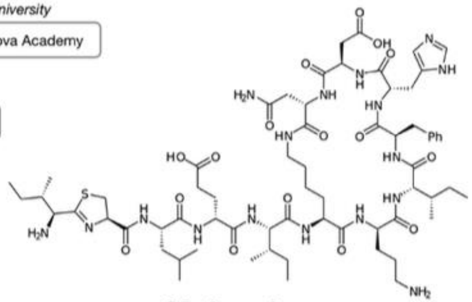
DNNs

A lot of real-world data does not “live” on grids

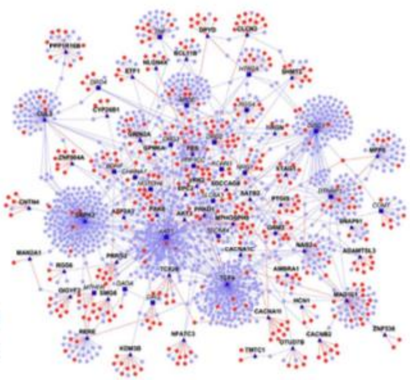
Knowledge graphs

Social networks
Citation networks
Communication networks
Multi-agent systems





Molecules



Protein interaction networks

Road maps

From CNN to GNN

* slide from Thomas Kipf, **University of Amsterdam**

Sequential Data

The teacher told the student that he was brilliant.

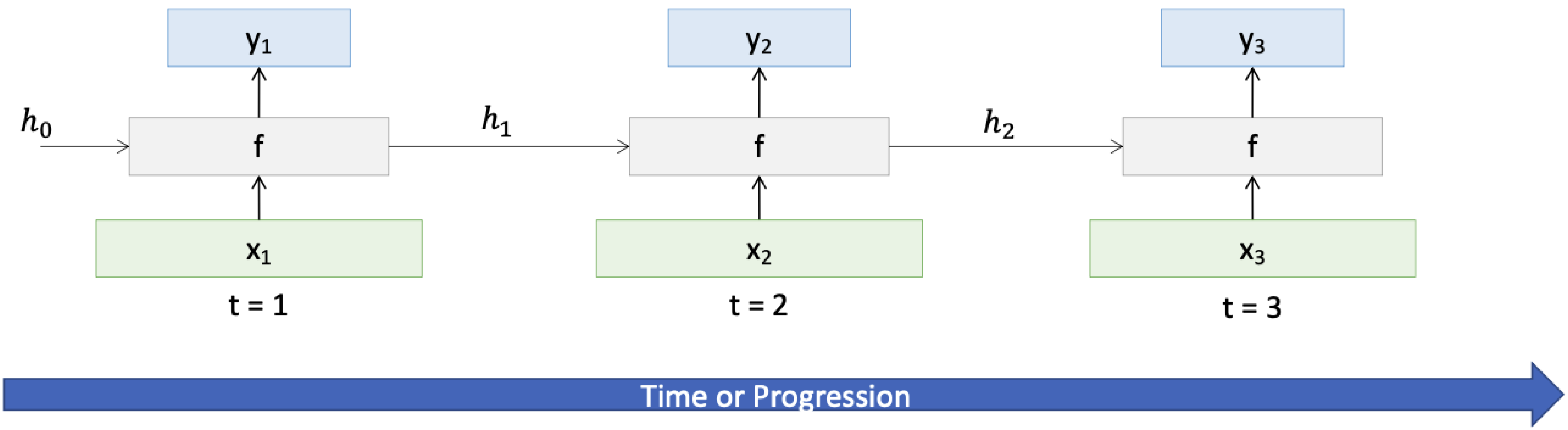
The student told the teacher that he was brilliant.

You read this sentence from left to right and

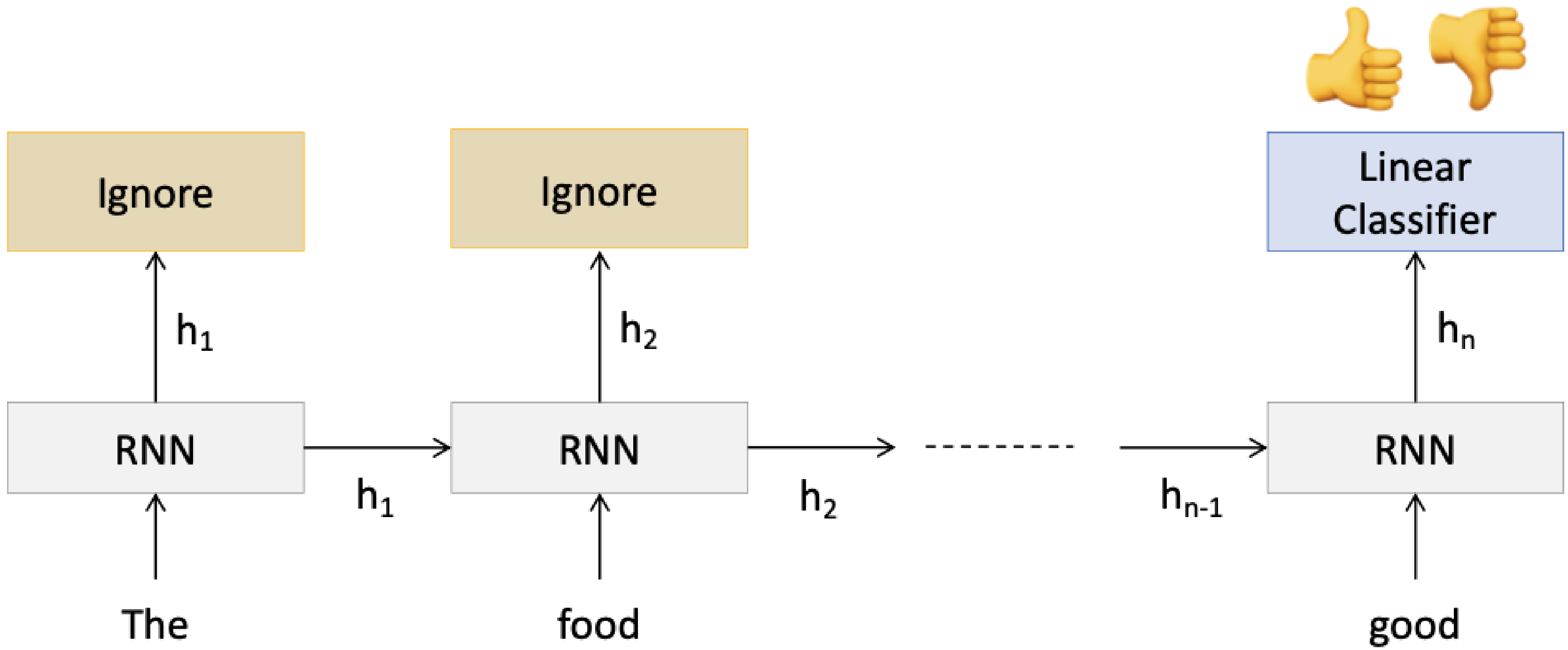
understand the sentence

Sequential Data - RNN

What if we have sequences of variable lengths, like sentences or videos that we would like to analyze?

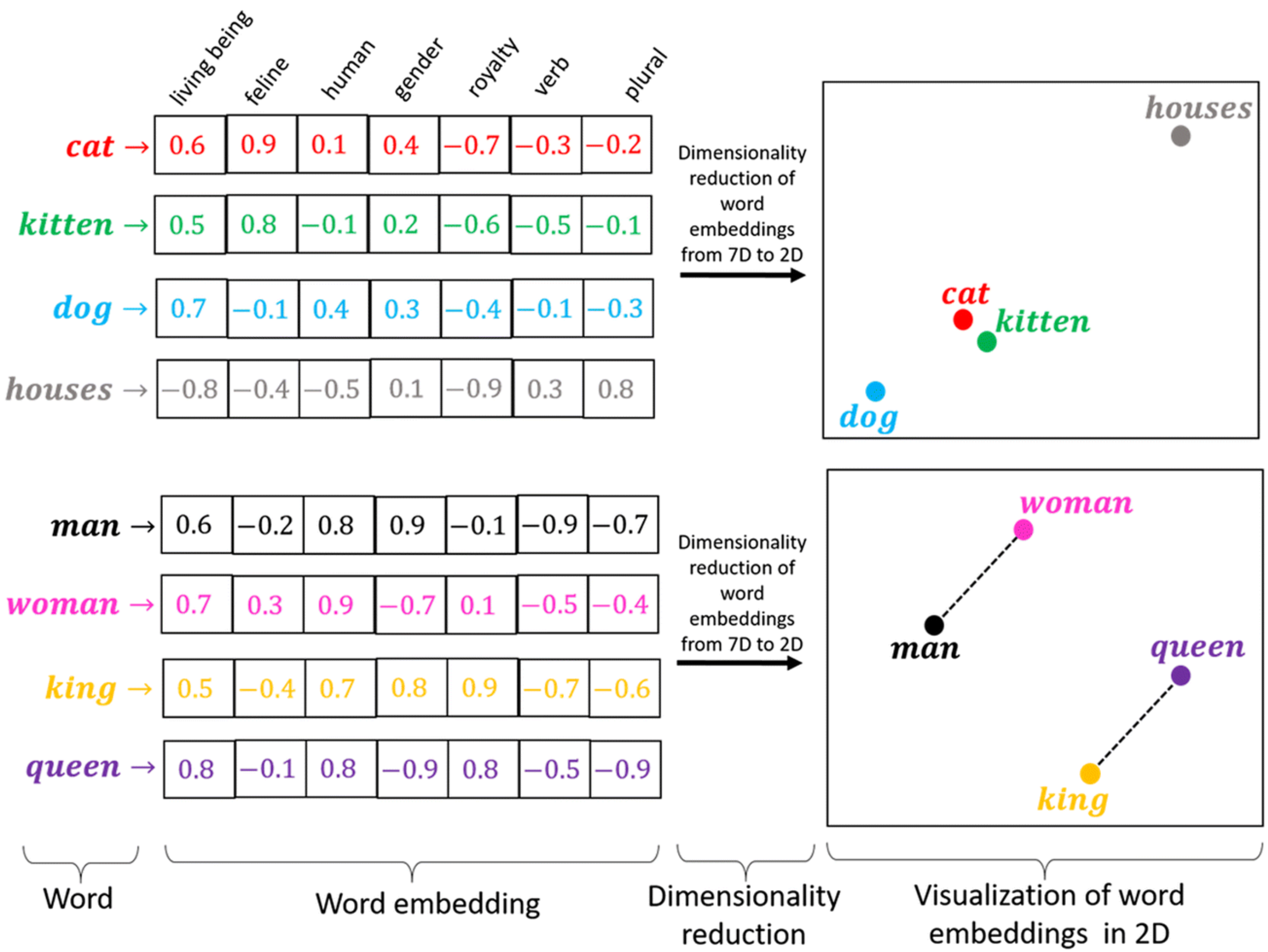


Sequential Data - RNN

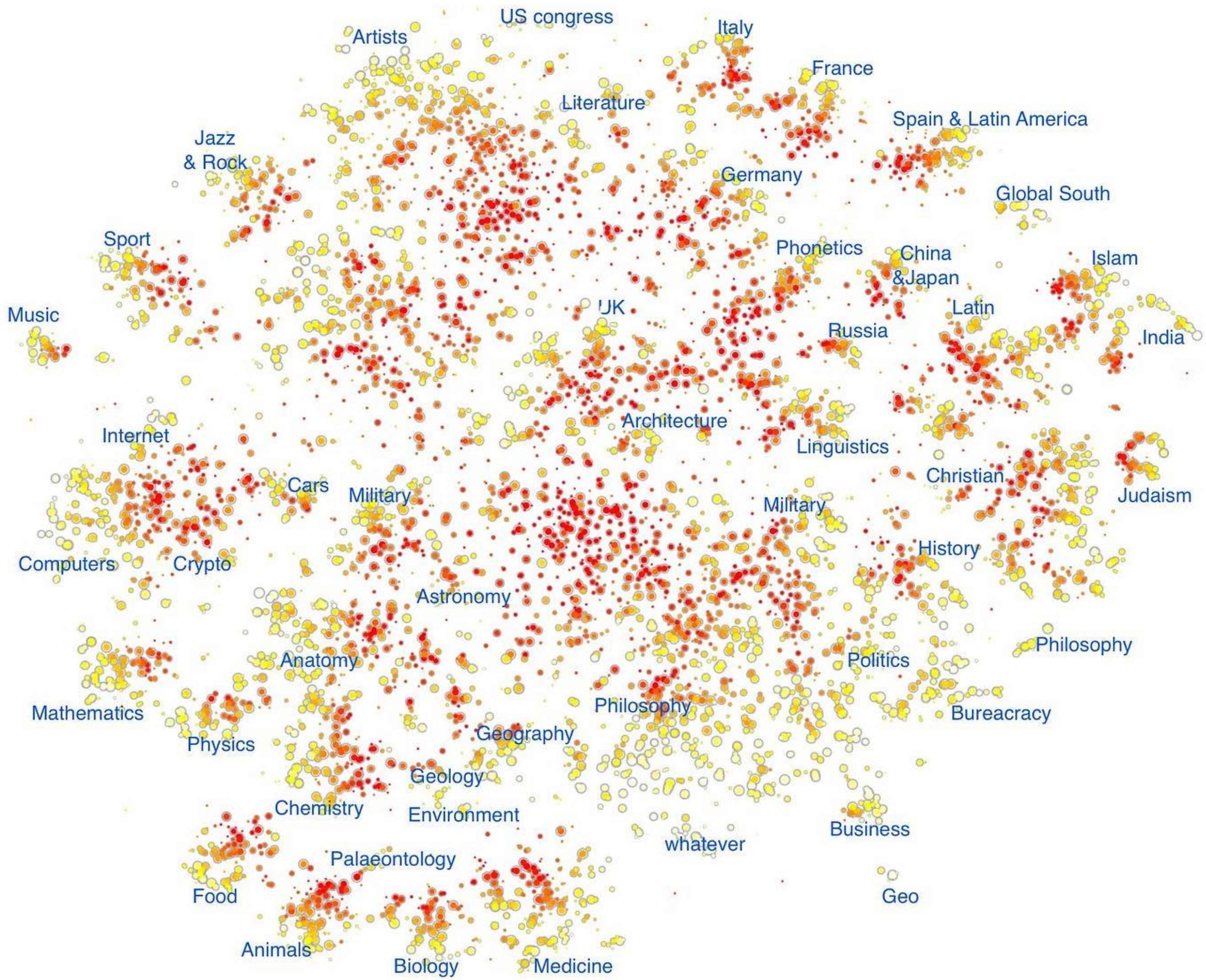


Token embedding –
DNA of the Token

Sequential Data - RNN

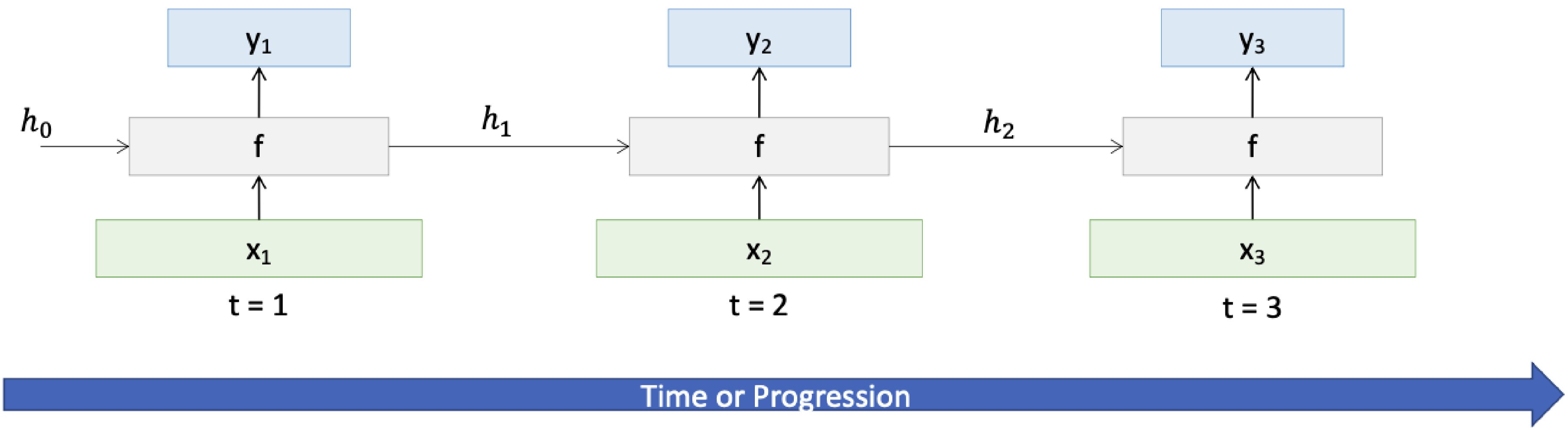


Sequential Data - RNN

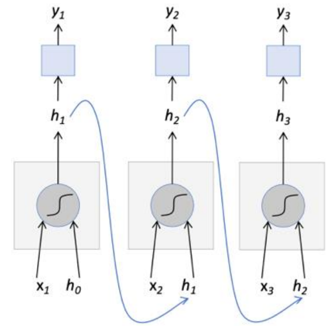


Sequential Data - RNN

What if we have sequences of variable lengths, like sentences or videos that we would like to analyze?

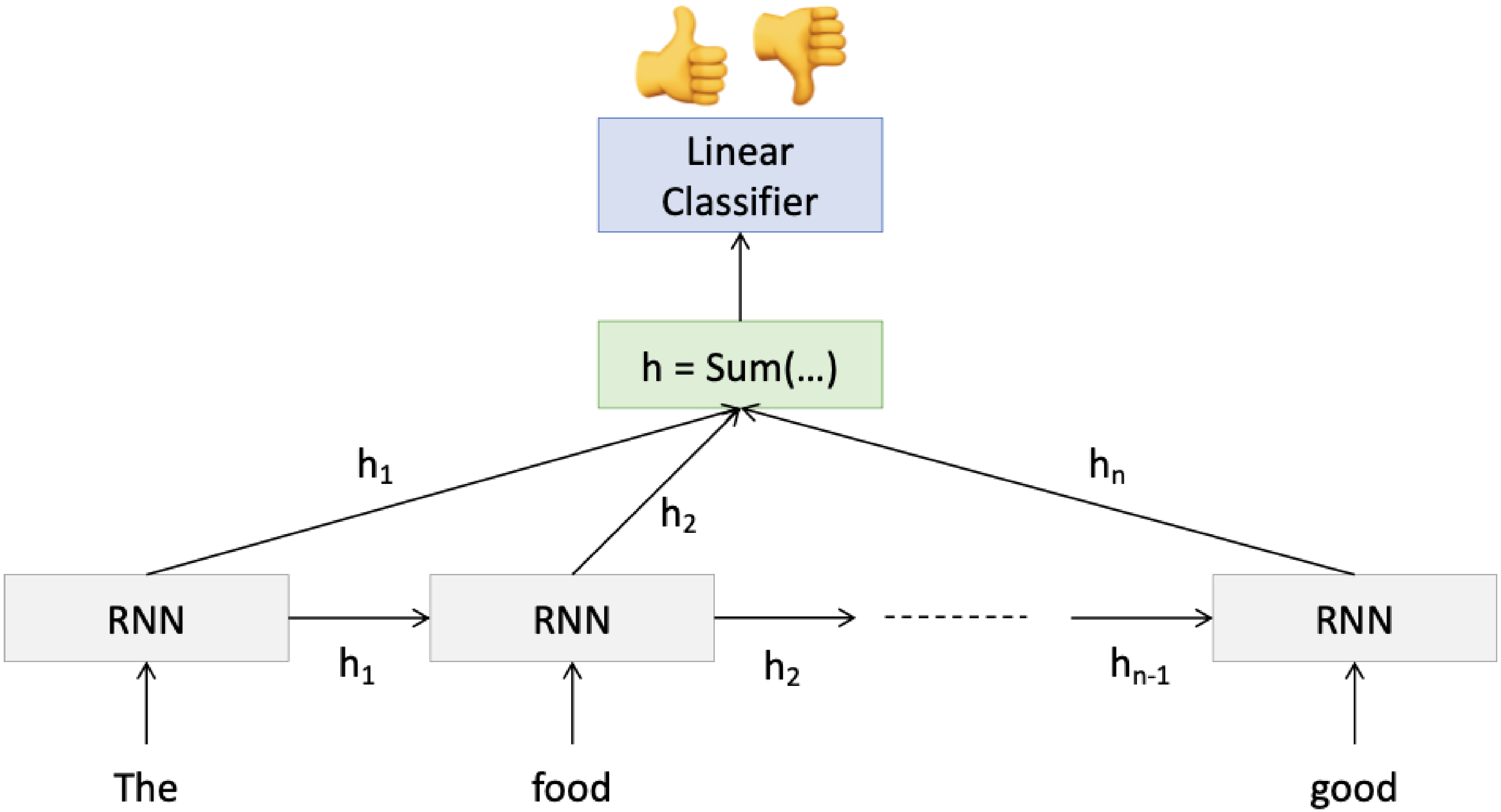


How would you setup the model (token embedding, MLP layer)



- $h_t = \sigma(W^T \begin{bmatrix} x_t \\ h_{t-1} \end{bmatrix})$
- $y_t = F(h_t)$

Sequential Data - RNN



Sequential Data - RNN

Image Captioning

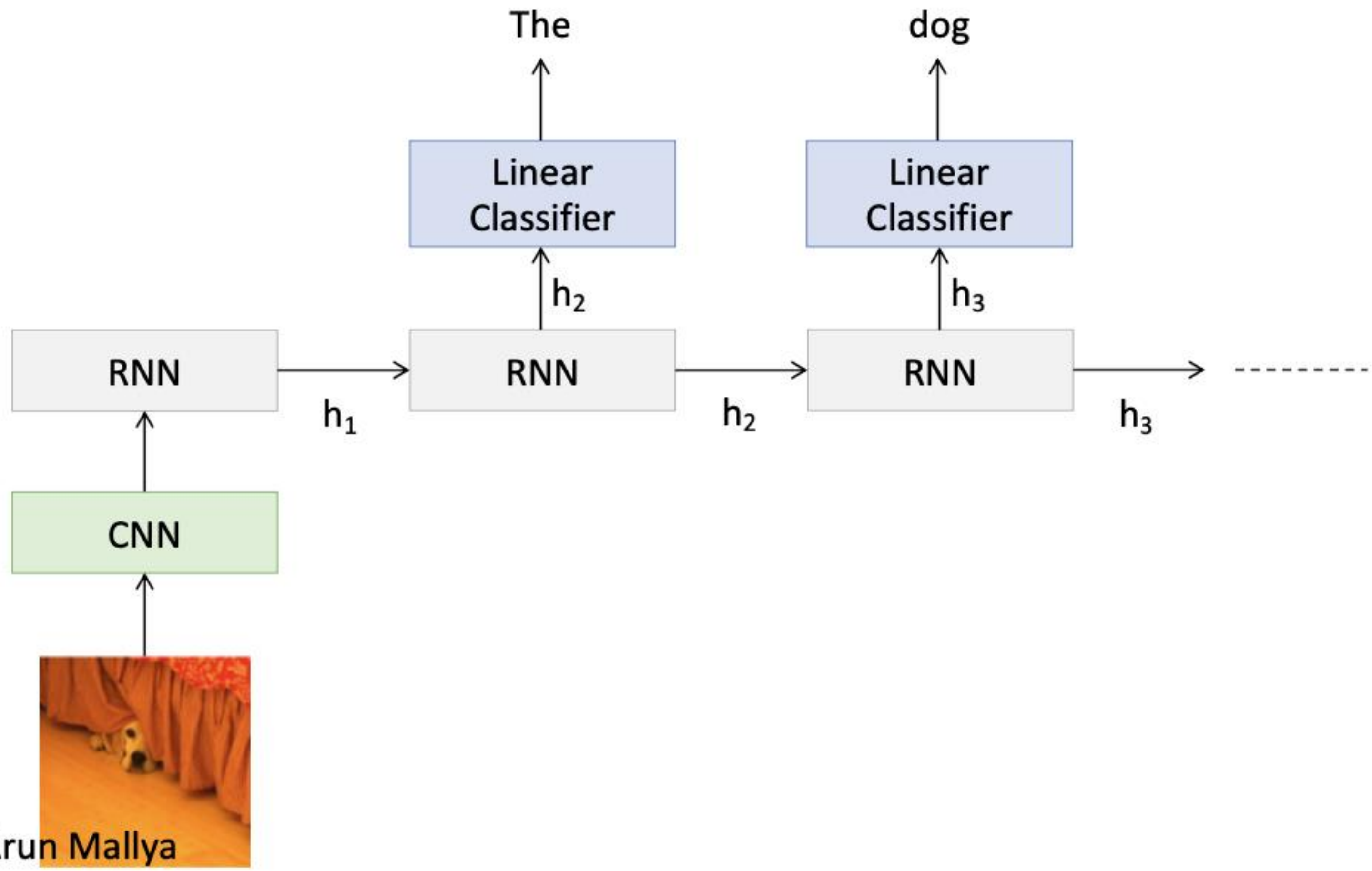
- Given an image, produce a sentence describing its contents

- Inputs: Image feature (from a CNN)
- Outputs: Multiple words (let's consider one sentence)

: The dog is hiding

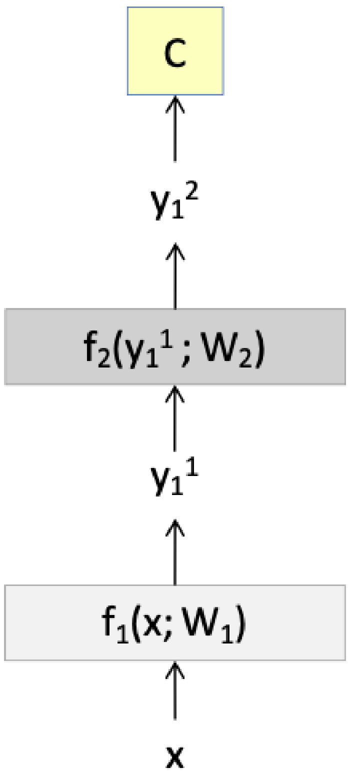
Sequential Data - RNN

Image Captioning



: Arun Mallya

Sequential Data - RNN



$$y_1 = f_1(x; W_1)$$

$$y_2 = f_2(y_1; W_2)$$

$$C = \text{Loss}(y_2, y_{GT})$$

$$\text{Find } \frac{\partial C}{\partial W_1}, \frac{\partial C}{\partial W_2}$$

$$\frac{\partial C}{\partial W_2} = \left(\frac{\partial C}{\partial y_2}\right)\left(\frac{\partial y_2}{\partial W_2}\right)$$

$$\frac{\partial C}{\partial W_1} = \left(\frac{\partial C}{\partial y_1}\right)\left(\frac{\partial y_1}{\partial W_1}\right)$$

$$= \left(\frac{\partial C}{\partial y_2}\right)\left(\frac{\partial y_2}{\partial y_1}\right)\left(\frac{\partial y_1}{\partial W_1}\right)$$

Sequential Data - RNN

$$h_t = f(Wh_{t-1} + b)$$

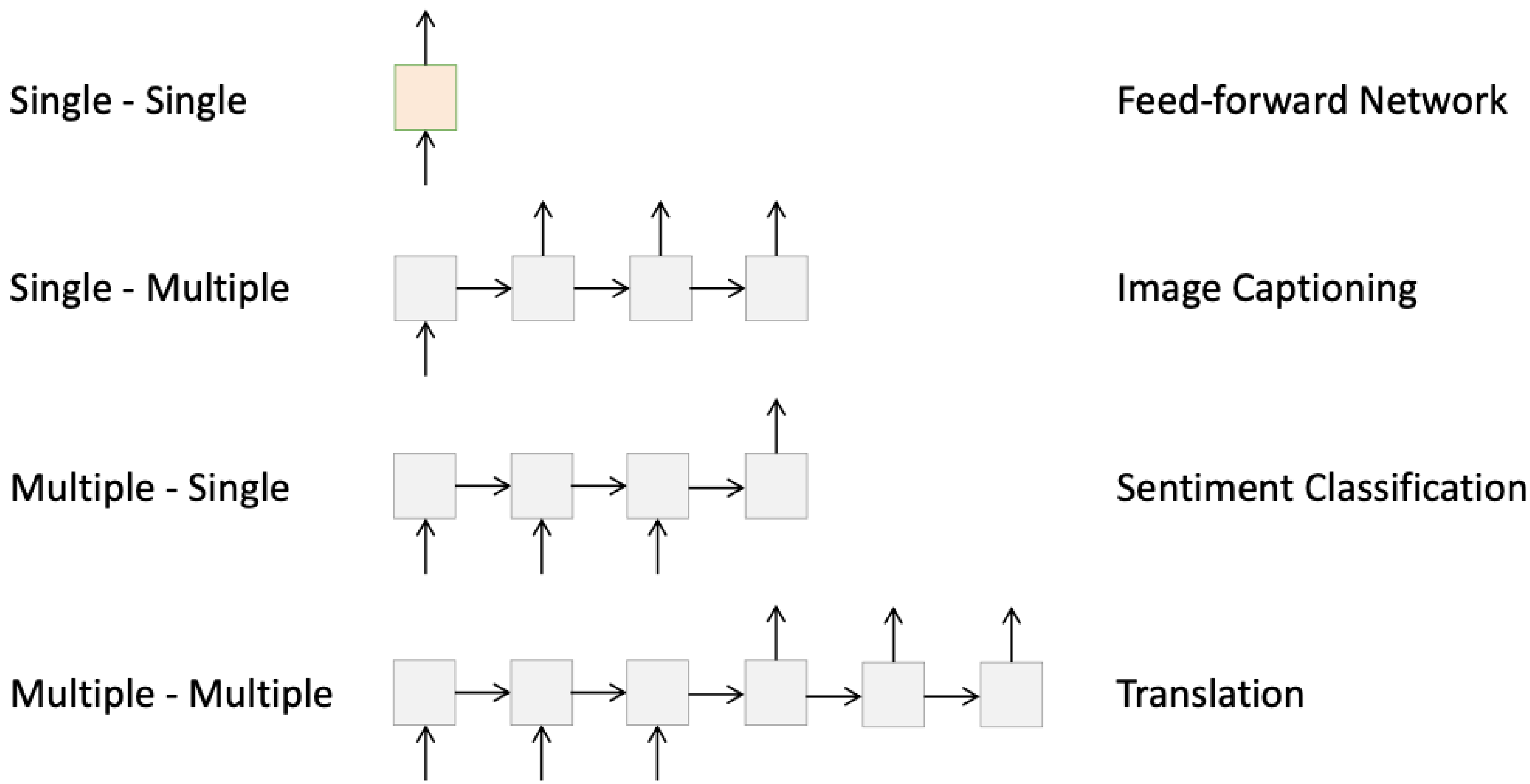
$$\|\frac{\partial L}{\partial h_0}\| \approx \sigma_{\max}^T \|\frac{\partial L}{\partial h_T}\|$$

- Largest singular value > 1 → **Exploding gradients**
  - Slight error in the late time steps causes drastic updates in the early time steps → Unstable learning
- Largest singular value < 1 → **Vanishing gradients**
  - Gradients passed to the early time steps is close to 0. → Uninformed correction

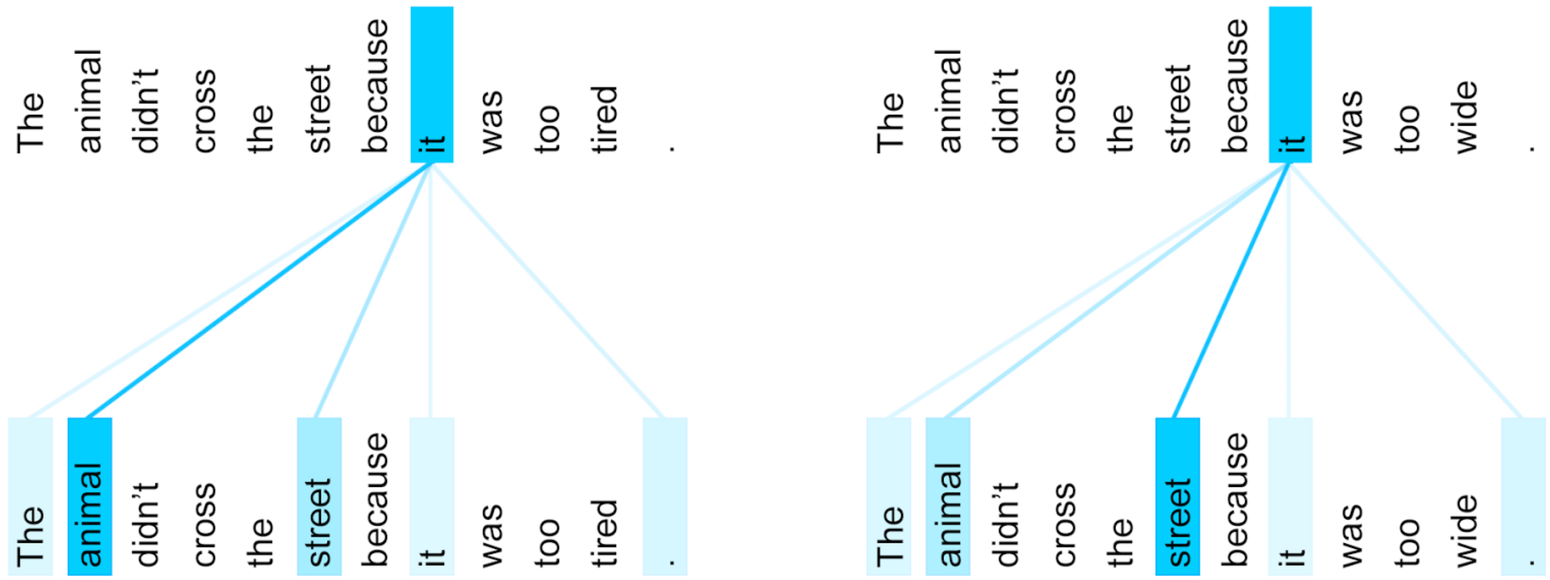
Any other problem with RNN?

Sequential Data - RNN

Input – Output Scenarios



Sequential Data - Transformer



Key **Value** **Query**

Sequential Data - Transformer

Think of YouTube.

First you enter your **Query** *in the search bar. Then your* **Query** *is compared against a set of* **Keys** *(in this case, video titles, tags and descriptions etc. within the YouTube database). After this, YouTube proceeds to retrieve the videos that best match your* **Query***. These video results are referred to as* **Values***.*

Key **Value** **Query**

I would like to taste the local food in France.

Sequential Data - Transformer

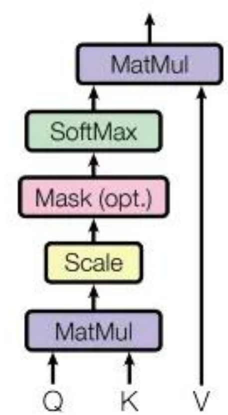
I would like to taste the local food in France.

$$Q = XW_Q \qquad K = XW_K \qquad V = XW_V$$

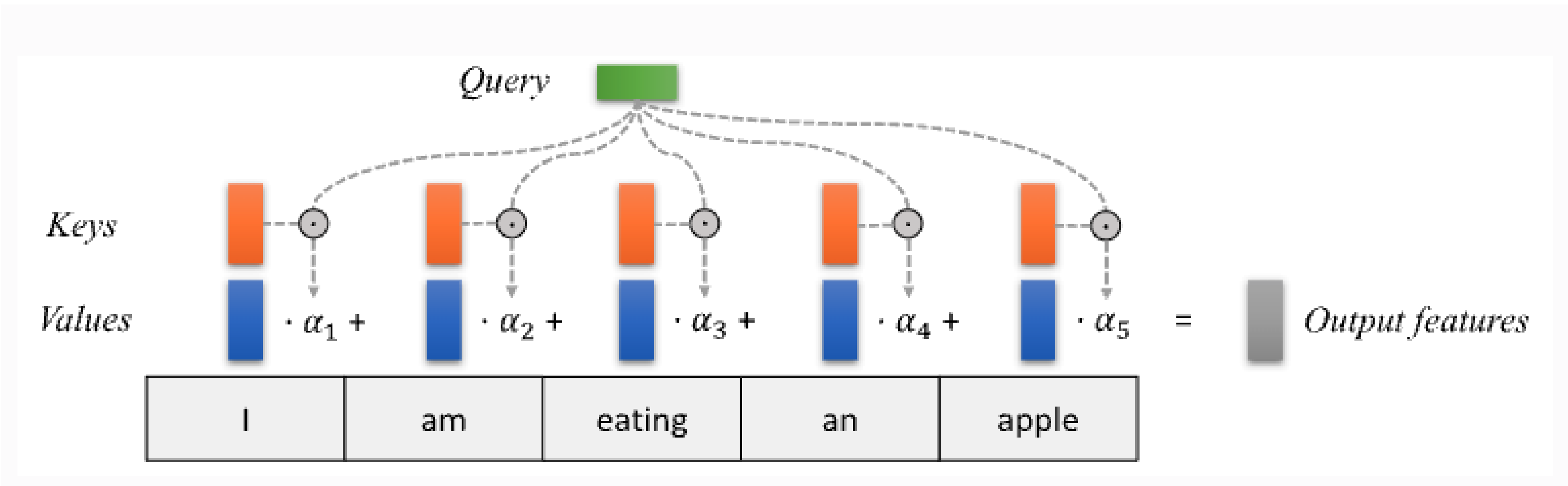
$$Q \cdot K = QK^T =$$

	I	would	like	to	taste	the	local	food	in	France
I	h									
would		h								
like			h							
to				h						
taste					h			h		
the						h				
local							h			h
food					h			h		
in									h	
France							h			h

$$softmax\left(\frac{Q_i K^T}{\sqrt{d_k}}\right) = \frac{e^{\left(\frac{Q_i K^T}{\sqrt{d_k}}\right)}}{\sum_{j=1}^{d_k} e^{\left(\frac{Q_j K^T}{\sqrt{d_k}}\right)}}$$



Sequential Data - Transformer

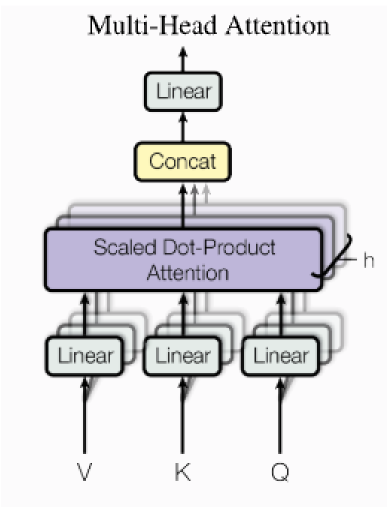


$$\alpha_i = \frac{\exp\left(f_{attn}\left(\text{key}_i, \text{query}\right)\right)}{\sum_j \exp\left(f_{attn}\left(\text{key}_j, \text{query}\right)\right)}, \quad \text{out} = \sum_i \alpha_i \cdot \text{value}_i$$

Sequential Data - Transformer

The scaled dot product attention allows a network to attend over a sequence. However, often there are multiple different aspects a sequence element wants to attend to, and a single weighted average is not a good option for it. This is why we extend the attention mechanisms to multiple heads

$$\mathrm{Multihead}(Q,K,V) = \mathrm{Concat}(\mathrm{head}_1,\ldots,\mathrm{head}_h)W^O$$
$$\text{where } \mathrm{head}_i = \mathrm{Attention}(QW_i^Q, KW_i^K, VW_i^V)$$



$W_{1\ldots h}^Q \in \mathbb{R}^{D\times d_k}, W_{1\ldots h}^K \in \mathbb{R}^{D\times d_k}, W_{1\ldots h}^V \in \mathbb{R}^{D\times d_v}$, and $W^O \in \mathbb{R}^{h\cdot d_v\times d_{out}}$

Sequential Data - Transformer

I would like to taste the local food in France.

$$Q = XW_Q \qquad K = XW_K \qquad V = XW_V$$

Self-Attention

Attention weight between the tokens corresponding to "Life" and "short"

	Life	is	short	eat	desert	first
Life	0.17	0.13	0.18	0.16	0.15	0.18
is	0.03	0.68	0.02	0.08	0.14	0.02
short	0.19	0.06	0.25	0.14	0.11	0.23
eat	0.15	0.21	0.14	0.16	0.17	0.14
desert	0.13	0.27	0.11	0.16	0.18	0.12
first	0.19	0.02	0.31	0.11	0.07	0.27

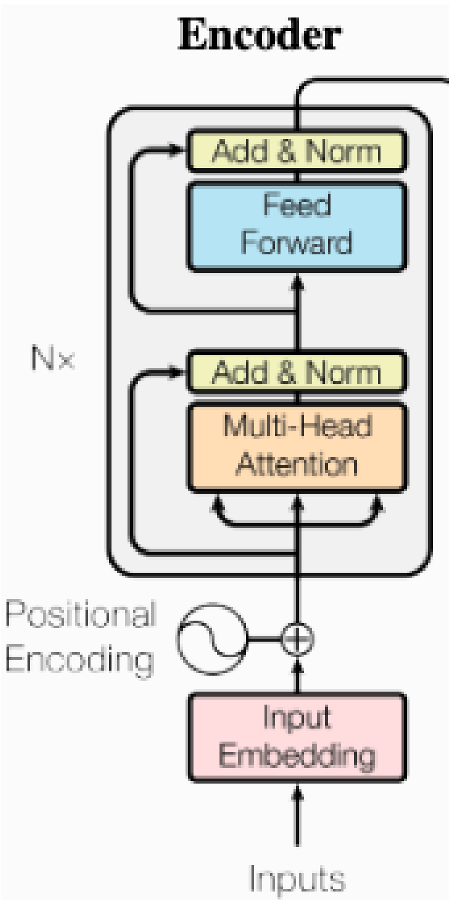
→

Causal-Attention

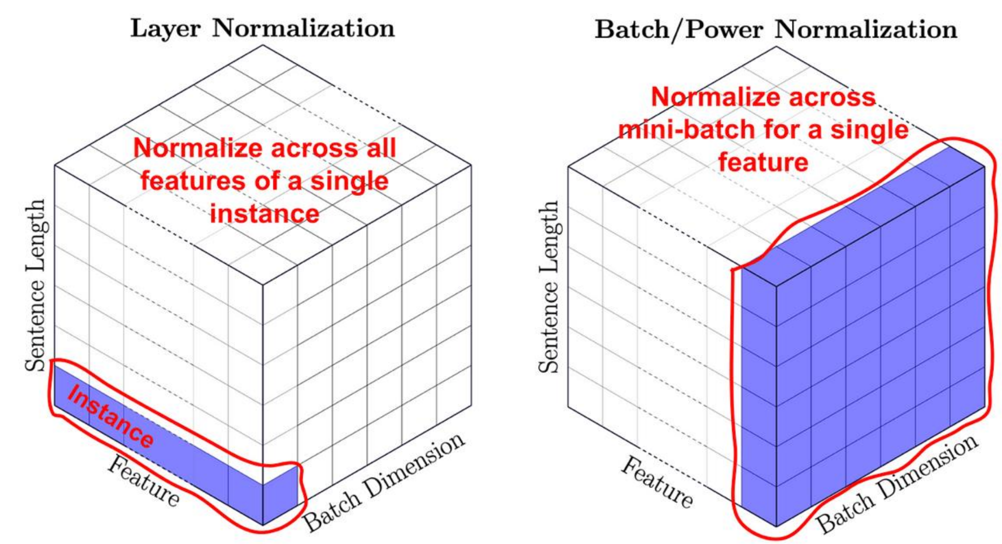
In the row for corresponding to "Life", mask out all words that come after "Life"

	Life	is	short	eat	desert	first
Life	0.17	0.13	0.18	0.16	0.15	0.18
is	0.03	0.68	0.02	0.08	0.14	0.02
short	0.19	0.06	0.25	0.14	0.11	0.23
eat	0.15	0.21	0.14	0.16	0.17	0.14
desert	0.13	0.27	0.11	0.16	0.18	0.12
first	0.19	0.02	0.31	0.11	0.07	0.27

Sequential Data - Transformer



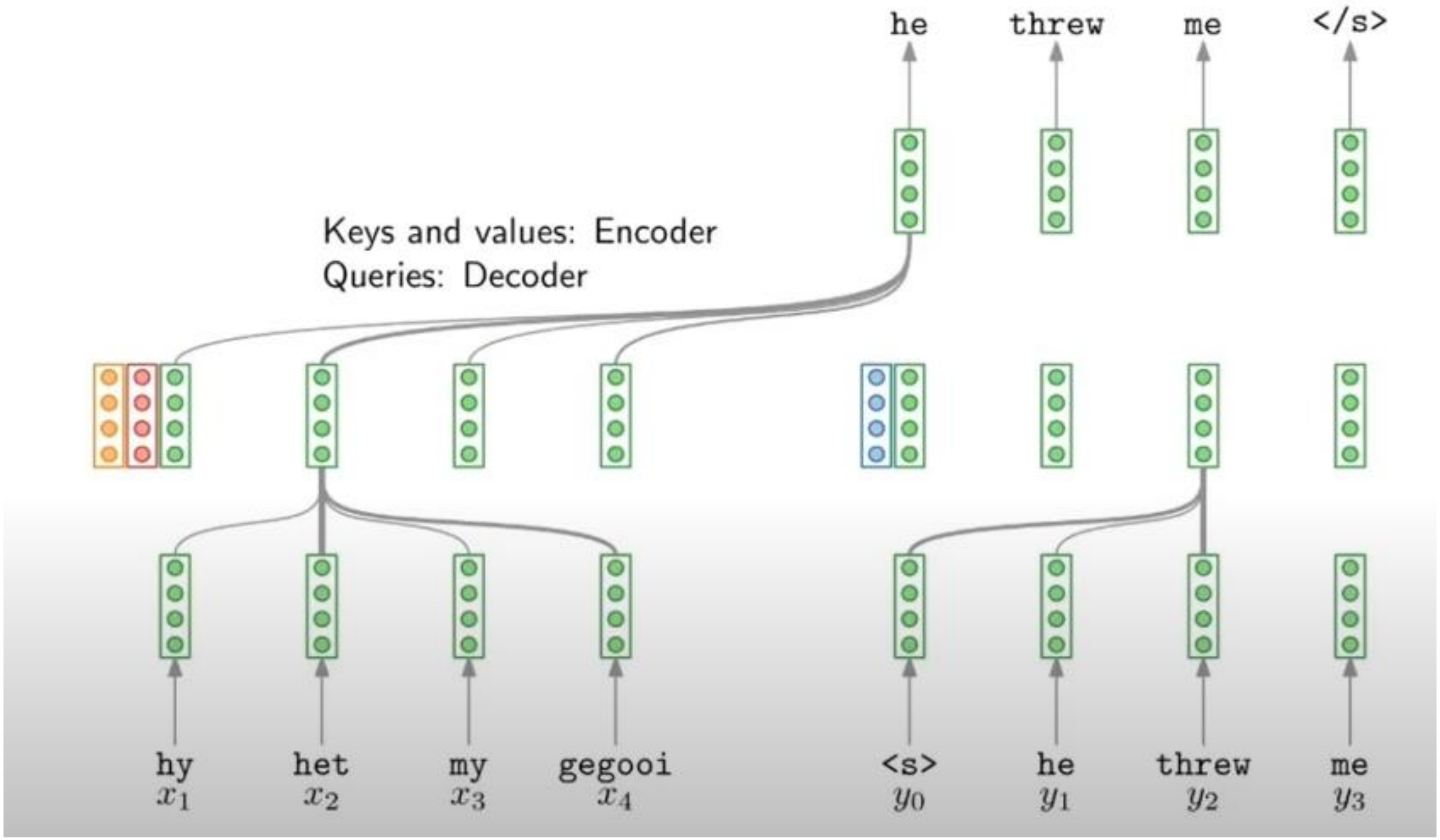
$$\mathrm{FFN}(x) = \max(0, xW_1 + b_1)W_2 + b_2$$
$$x = \mathrm{LayerNorm}(x + \mathrm{FFN}(x))$$



$$\mu^l = \frac{1}{H}\sum_{i=1}^{H} a_i^l \qquad \sigma^l = \sqrt{\frac{1}{H}\sum_{i=1}^{H}\left(a_i^l - \mu^l\right)^2}$$

Sequential Data - Transformer

Cross-attention



Sequential Data - Transformer

Multi-Attention

Self-Attention | **Causal-Attention** | **Cross-Attention**

Sentiment Analysis	Next-token Prediction	Translation

Sequential Data - Transformer

The teacher told the student that he was brilliant.

The student told the teacher that he was brilliant.

Two sentences using exactly the same tokens but end up with very different meaning

Sequential Data - Transformer

0 :	0	0	0	0	8 :	1	0	0	0
1 :	0	0	0	1	9 :	1	0	0	1
2 :	0	0	1	0	10 :	1	0	1	0
3 :	0	0	1	1	11 :	1	0	1	1
4 :	0	1	0	0	12 :	1	1	0	0
5 :	0	1	0	1	13 :	1	1	0	1
6 :	0	1	1	0	14 :	1	1	1	0
7 :	0	1	1	1	15 :	1	1	1	1

Sequential Data - Transformer

$$P(k, 2i) = \sin\left(\frac{k}{n^{2i/d}}\right)$$

$$P(k, 2i+1) = \cos\left(\frac{k}{n^{2i/d}}\right)$$

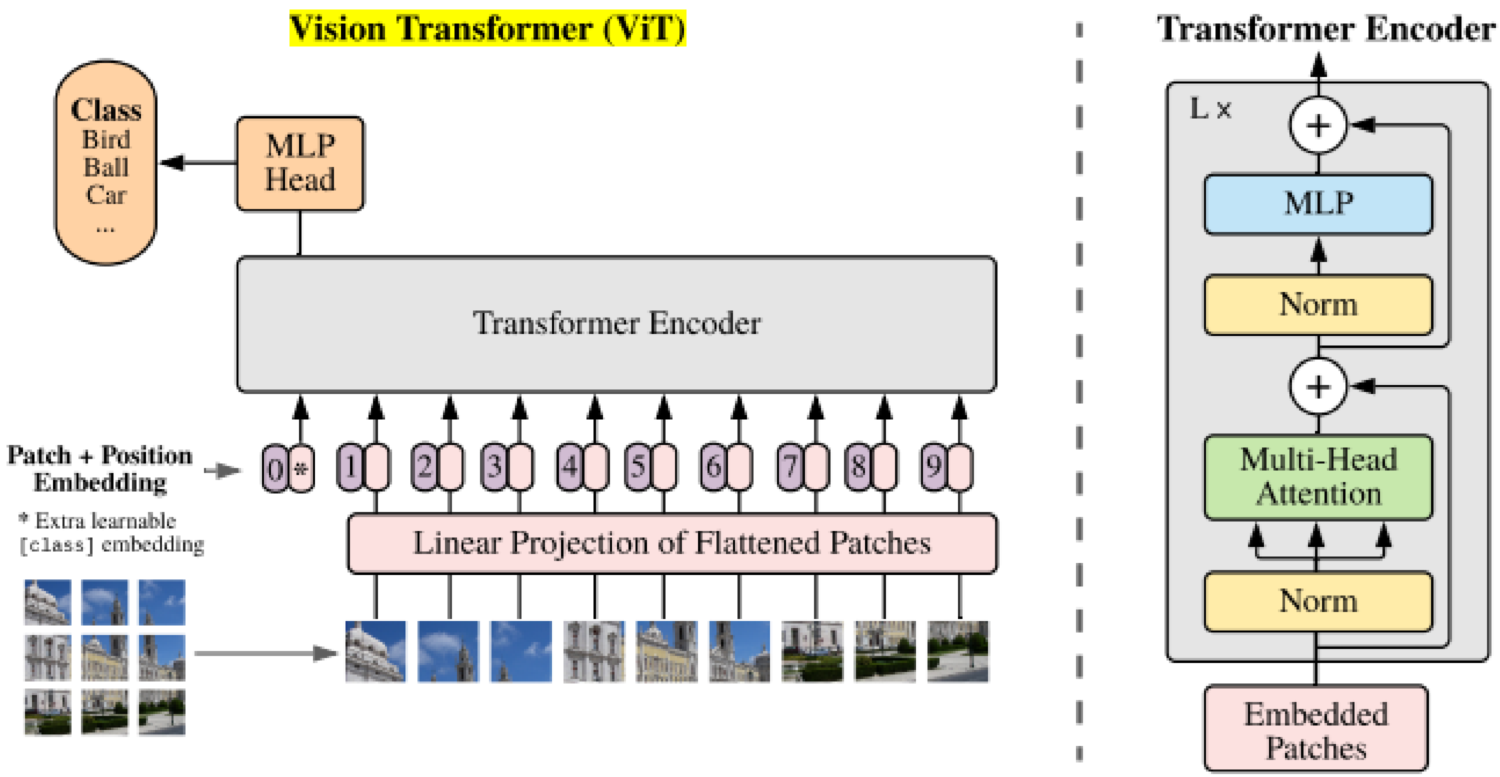
k: Position of an object in the input sequence,

d: Dimension of the output embedding space

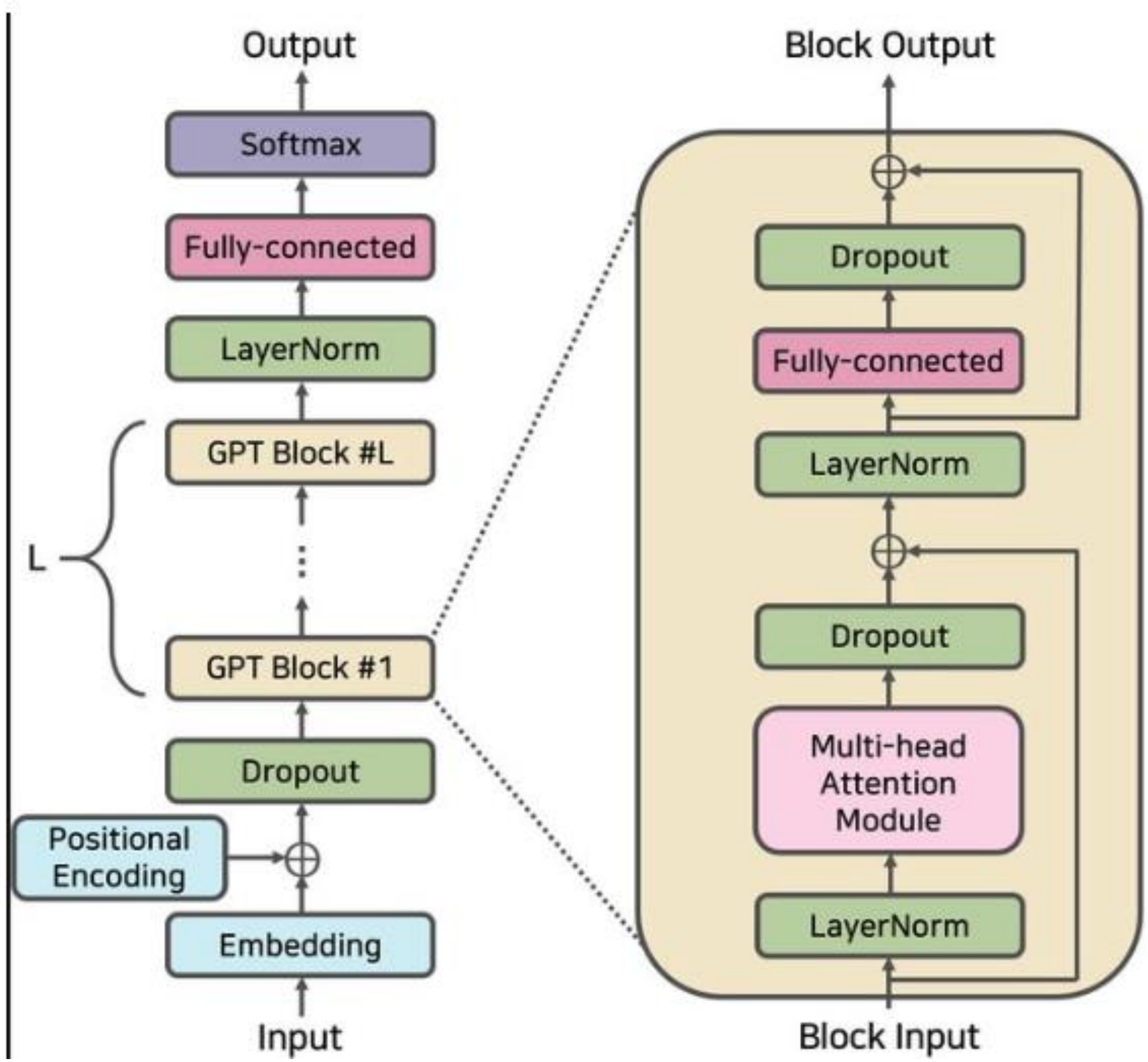
Positional Encoding Matrix with d=4, n=100

Sequence	Index of token, k	i=0	i=0	i=1	i=1
I	0	P_{00}=sin(0) = 0	P_{01}=cos(0) = 1	P_{02}=sin(0) = 0	P_{03}=cos(0) = 1
am	1	P_{10}=sin(1/1) = 0.84	P_{11}=cos(1/1) = 0.54	P_{12}=sin(1/10) = 0.10	P_{13}=cos(1/10) = 1.0
a	2	P_{20}=sin(2/1) = 0.91	P_{21}=cos(2/1) = -0.42	P_{22}=sin(2/10) = 0.20	P_{23}=cos(2/10) = 0.98
Robot	3	P_{30}=sin(3/1) = 0.14	P_{31}=cos(3/1) = -0.99	P_{32}=sin(3/10) = 0.30	P_{33}=cos(3/10) = 0.96

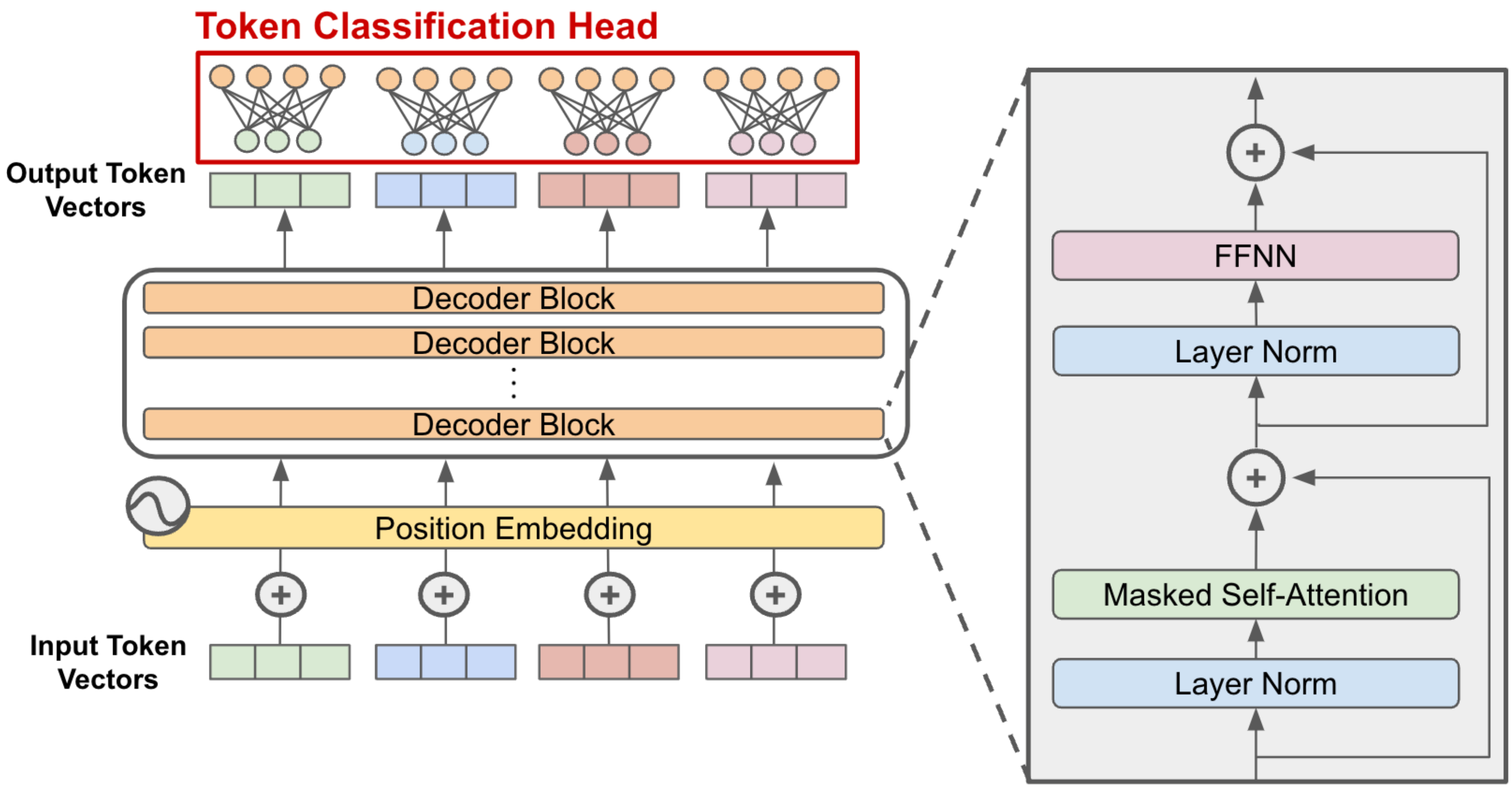
Sequential Data – Vision Transformer



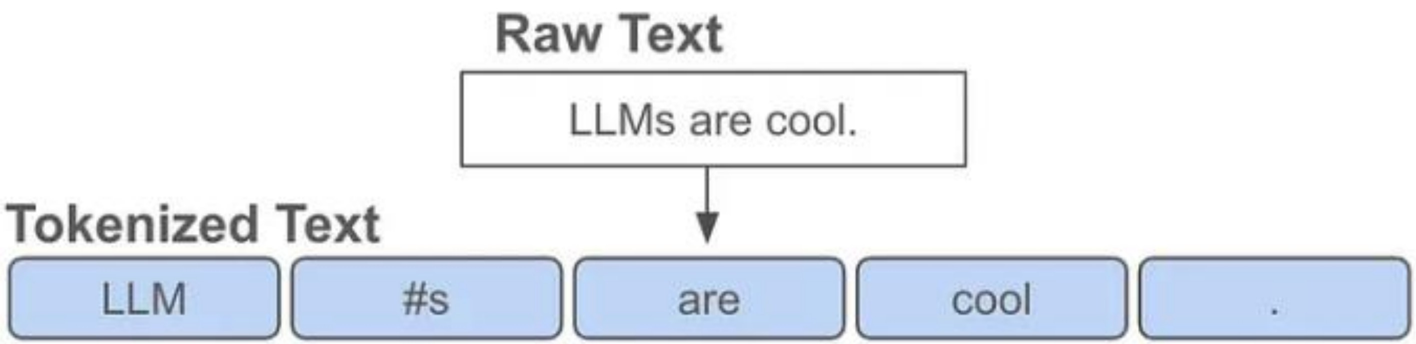
Sequential Data – GPT Transformer

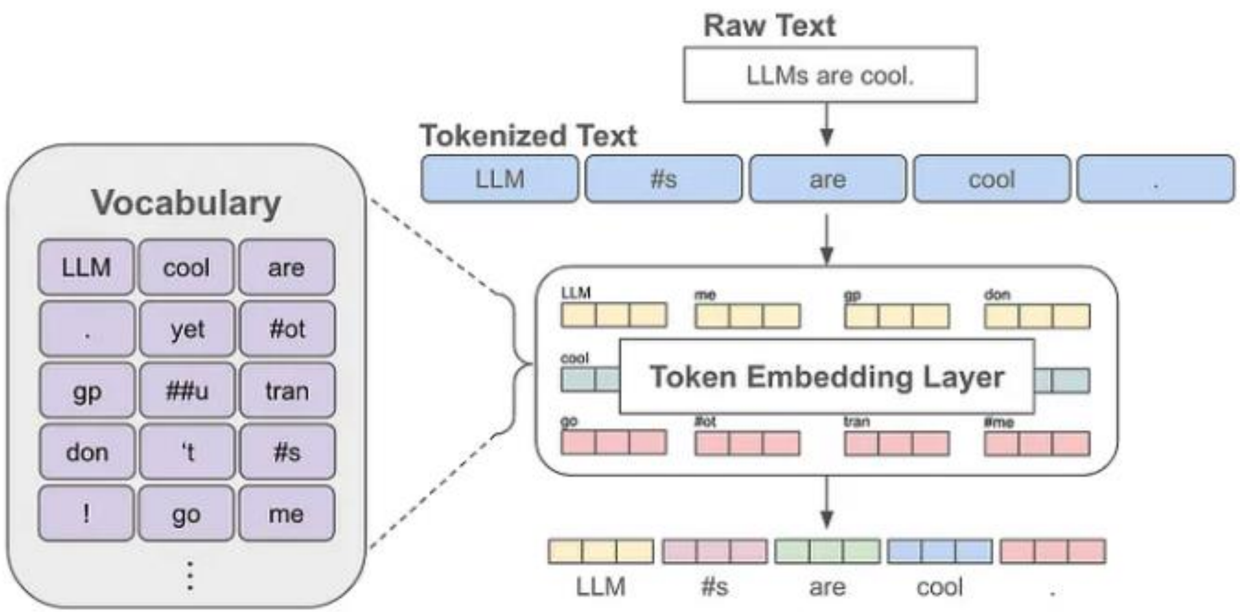


Sequential Data - Transformer

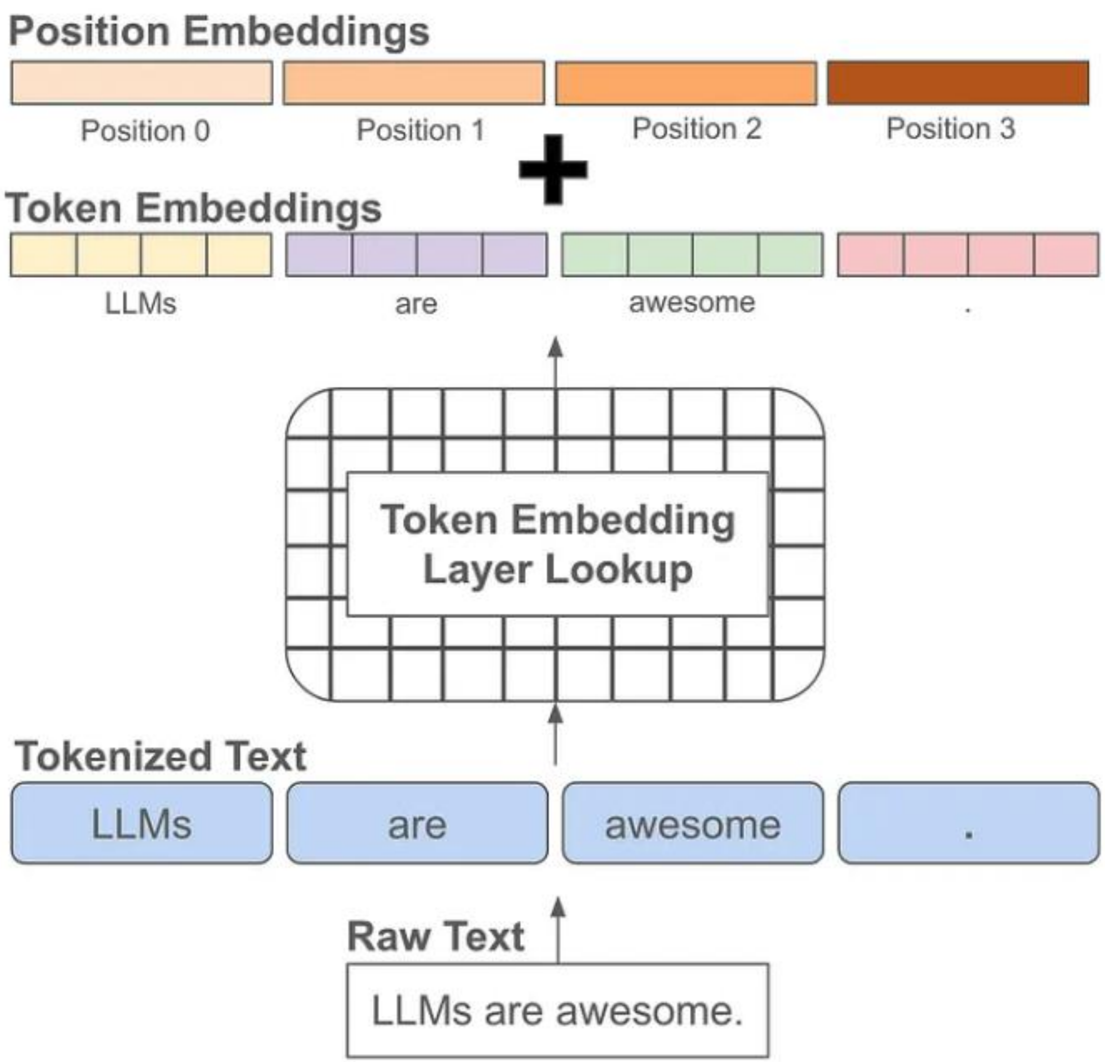


Sequential Data - Transformer



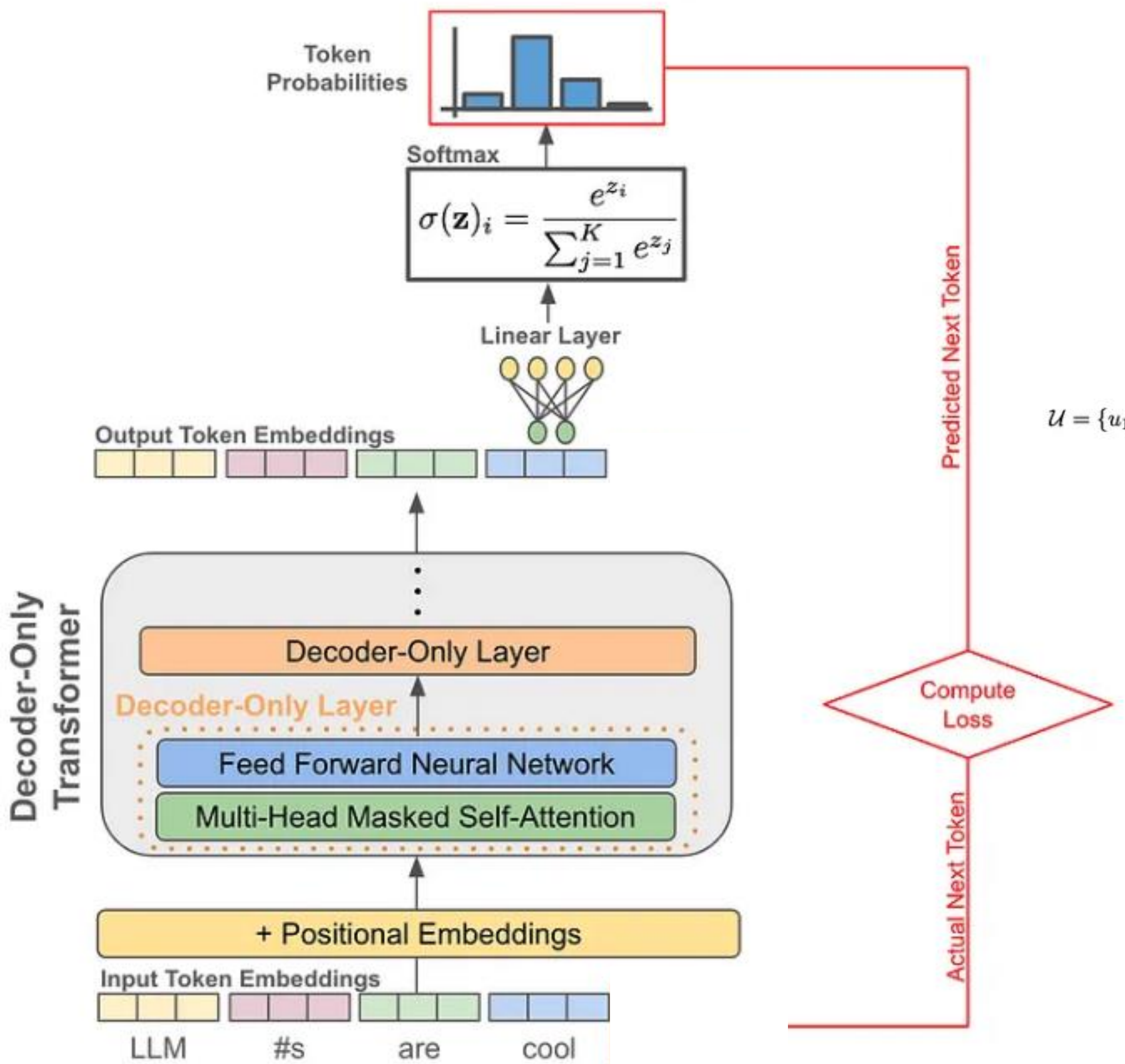


Sequential Data - Transformer



Position Embeddings With In a Language Model

Sequential Data – Transformer - Training

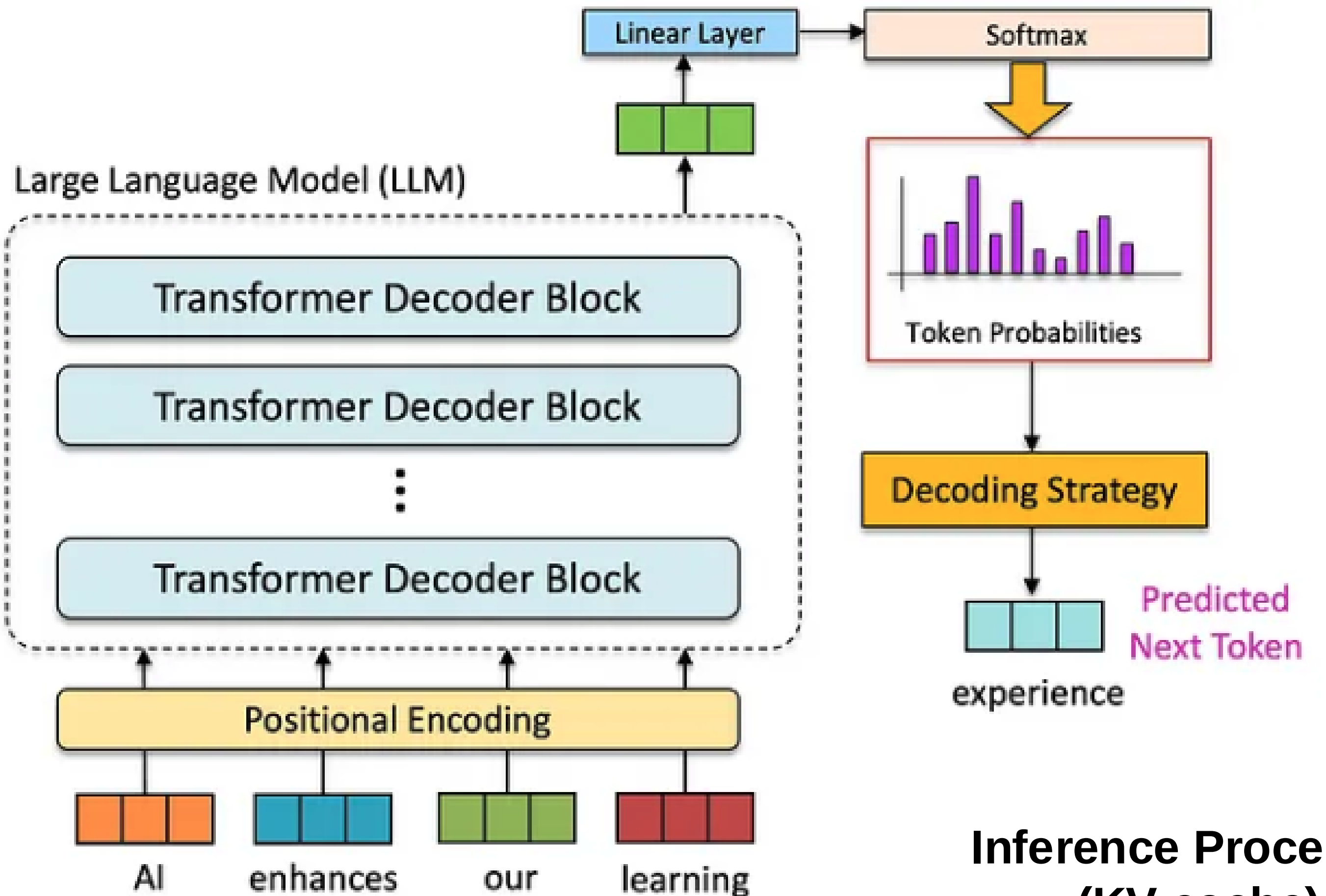


Training Procedure

$$\mathcal{U} = \{u_1, u_2, \ldots, u_N\}$$

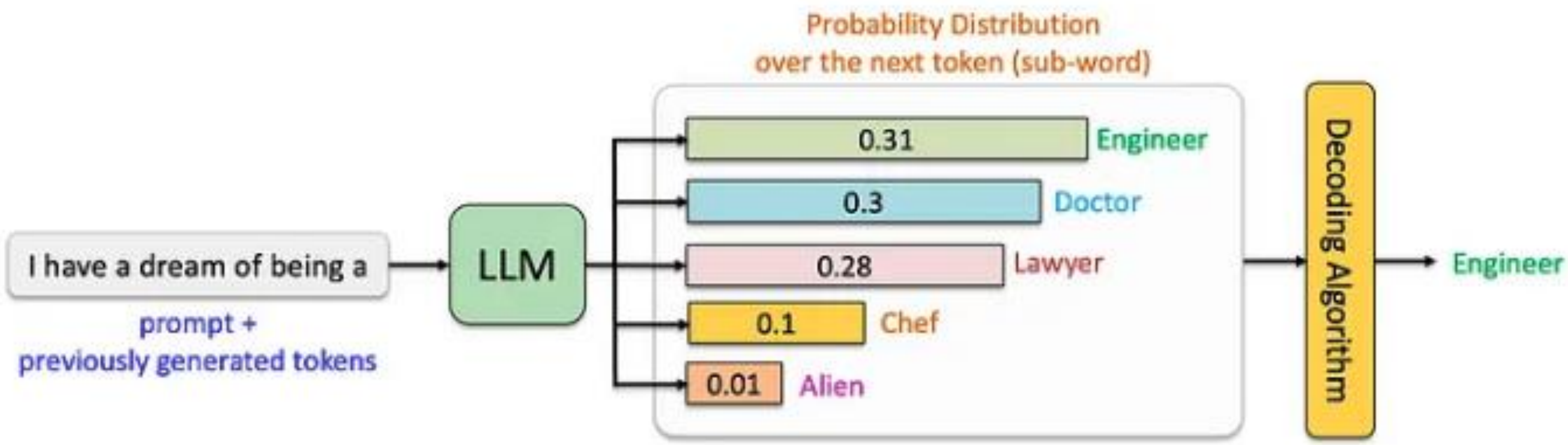
$$\underbrace{\mathcal{L}(\mathcal{U})}_{\text{Language model loss over the full text corpus}} = \sum_{i=1}^{N} \log \underbrace{\left(\mathbb{P}(u_i | u_{i-k}, \ldots, u_{i-1}, \Theta)\right)}_{\text{Conditional probability of i-th token given k preceding tokens and model parameters } \theta}$$

Sequential Data – Transformer - Inference



Inference Procedure (KV cache)

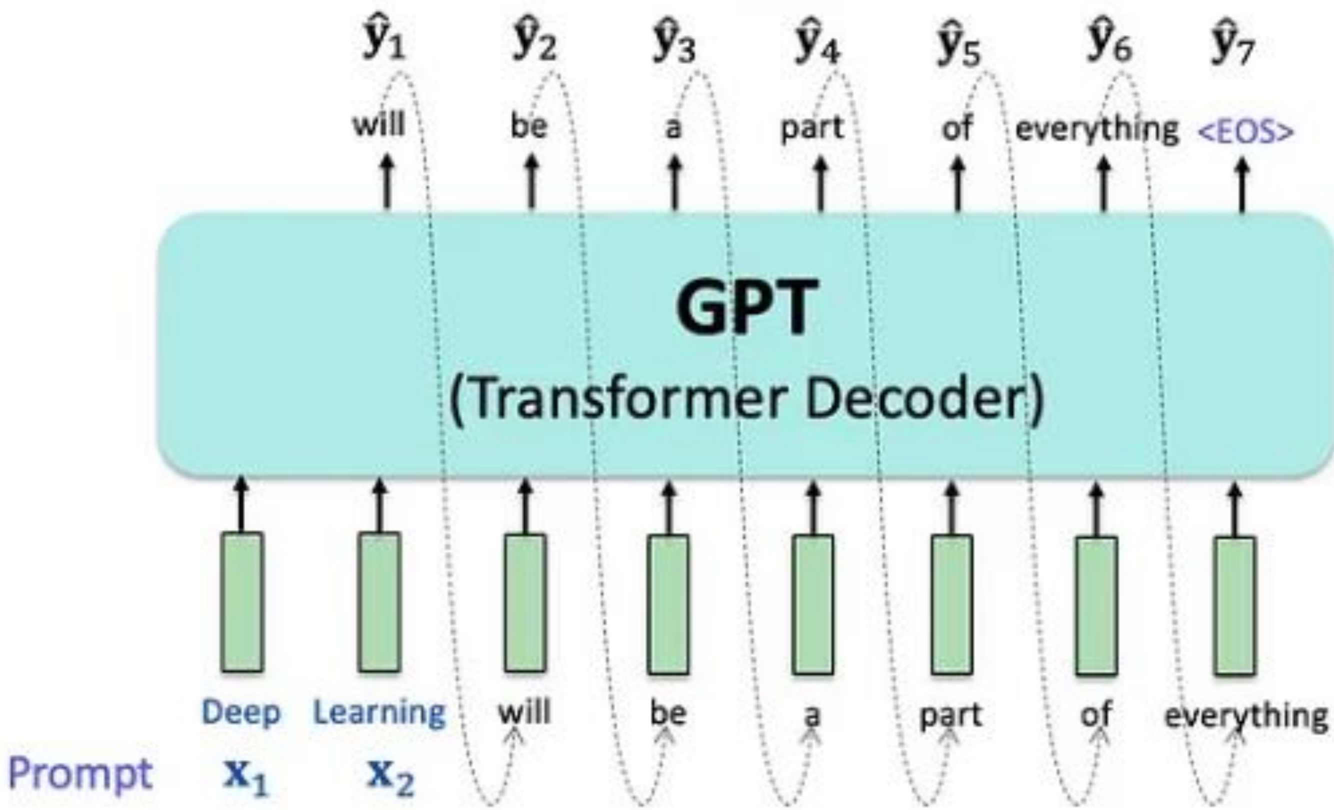
Sequential Data – Transformer - Inference



Autoregressive Nature

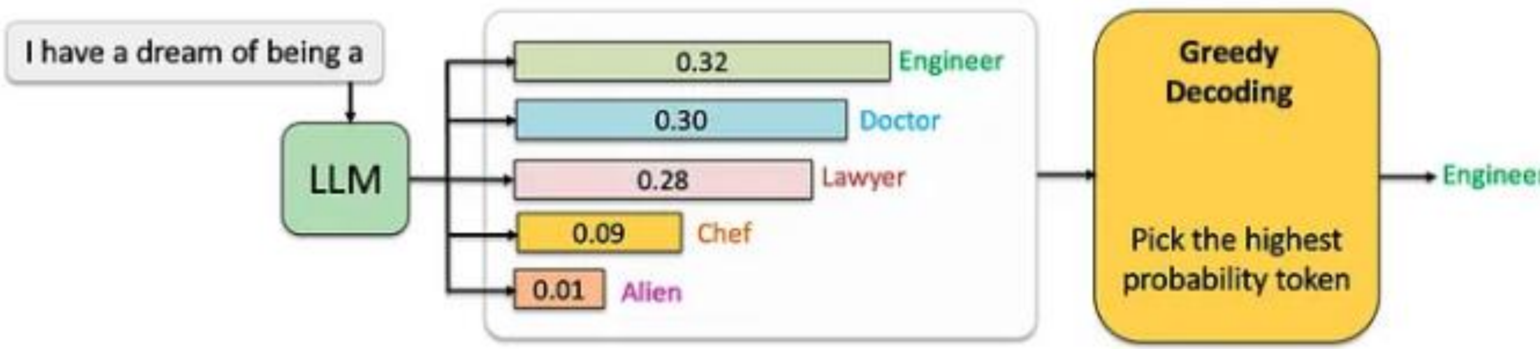
$$P(\hat{\mathbf{y}}_i | \mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m, \hat{\mathbf{y}}_1, \hat{\mathbf{y}}_2, \dots, \hat{\mathbf{y}}_{i-1})$$

Sequential Data – Transformer - Inference



Sequential Data – Transformer - Inference

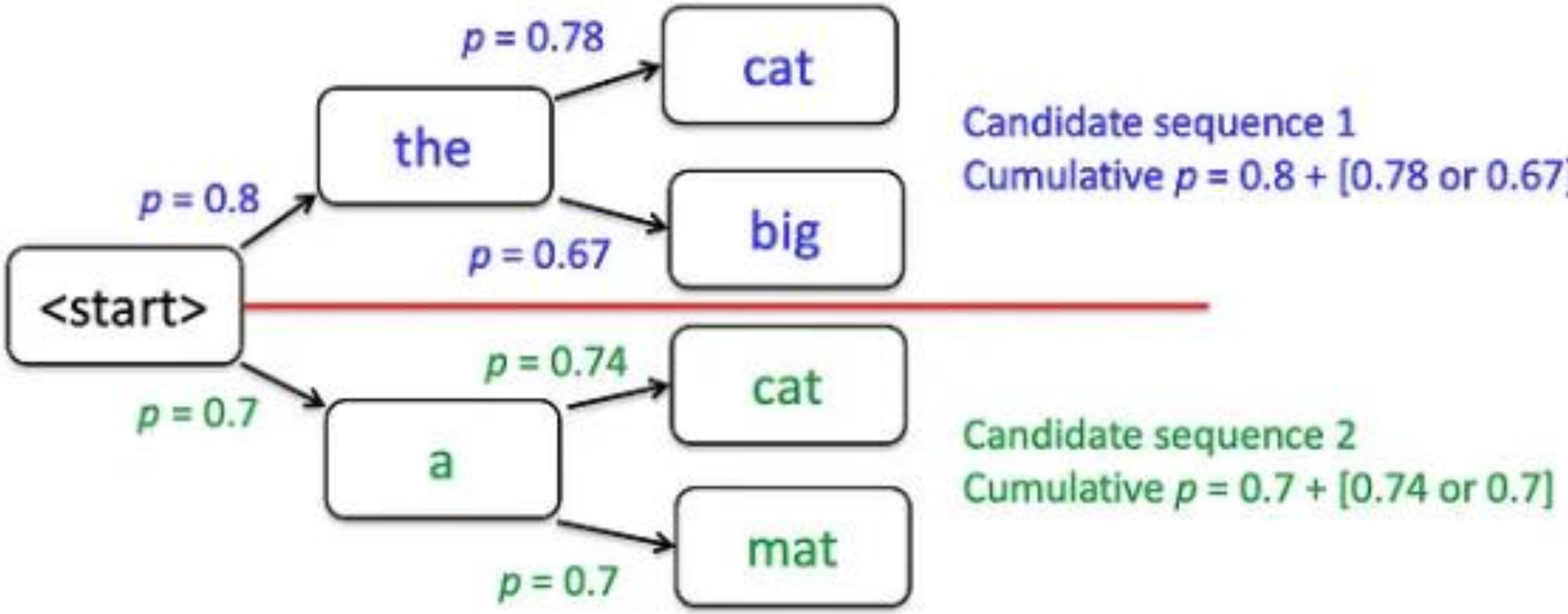
$$\hat{\mathbf{y}}_i = \arg\max_{\hat{\mathbf{y}}} P(\hat{\mathbf{y}}|\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_m, \hat{\mathbf{y}}_1, \hat{\mathbf{y}}_2, \ldots, \hat{\mathbf{y}}_{i-1})$$



Greedy Decoding

Greedy decoding is computationally efficient and easy to implement.
It does not explore alternative paths that might lead to more globally optimal sequences.

Sequential Data – Transformer - Inference



https://medium.com/@lmpo/mastering-llms-a-guide-to-decoding-algorithms-c90a48fd167b

DNNs

Deep Neural Networks

20^{th} Century Zoo of Neural Network Architectures