CS540 Introduction to Artificial Intelligence

Neural Networks: Review

University of Wisconsin-Madison

Spring 2024

Announcements

- **Homework:**
  - HW7 is due on **Thursday Apr. 4 at 11 AM**
- Class roadmap:

Tuesday, Apr. 2	Deep Learning and Neural Network's Summary
Thursday, Apr. 4	Search I: Un-Informed search
Tuesday, Apr. 9	Search II: Informed search

How to classify

Cats vs. dogs?

Single-layer Perceptron

↓

Multi-layer Perceptron

↓

Training of neural networks

↓

Convolutional neural networks

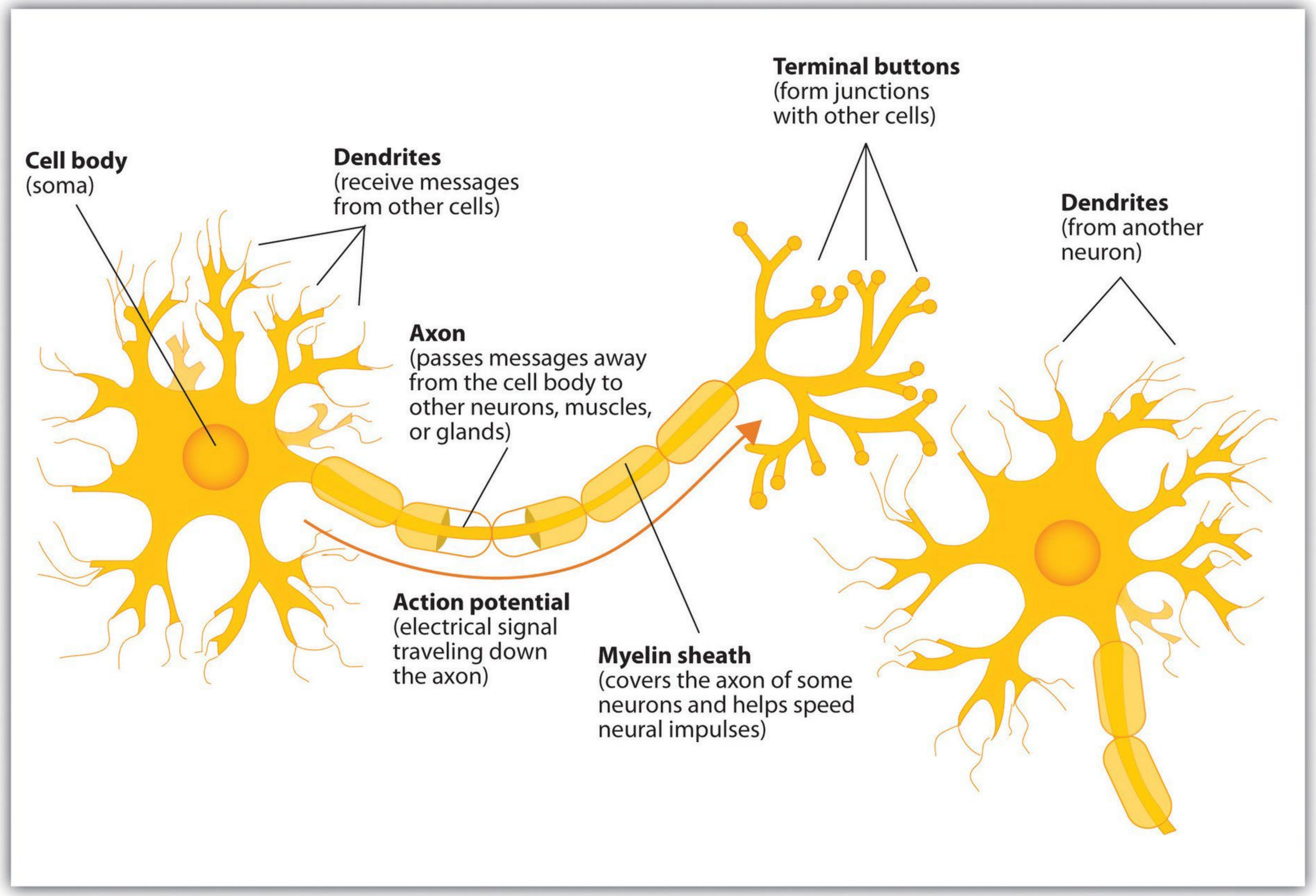
Neural networks can also be used for regression.

- Typically, no activation on outputs, mean squared error loss function.

Inspiration from neuroscience

- Inspirations from human brains
- Networks of simple and homogenous units (a.k.a **neuron**)

(wikipedia)



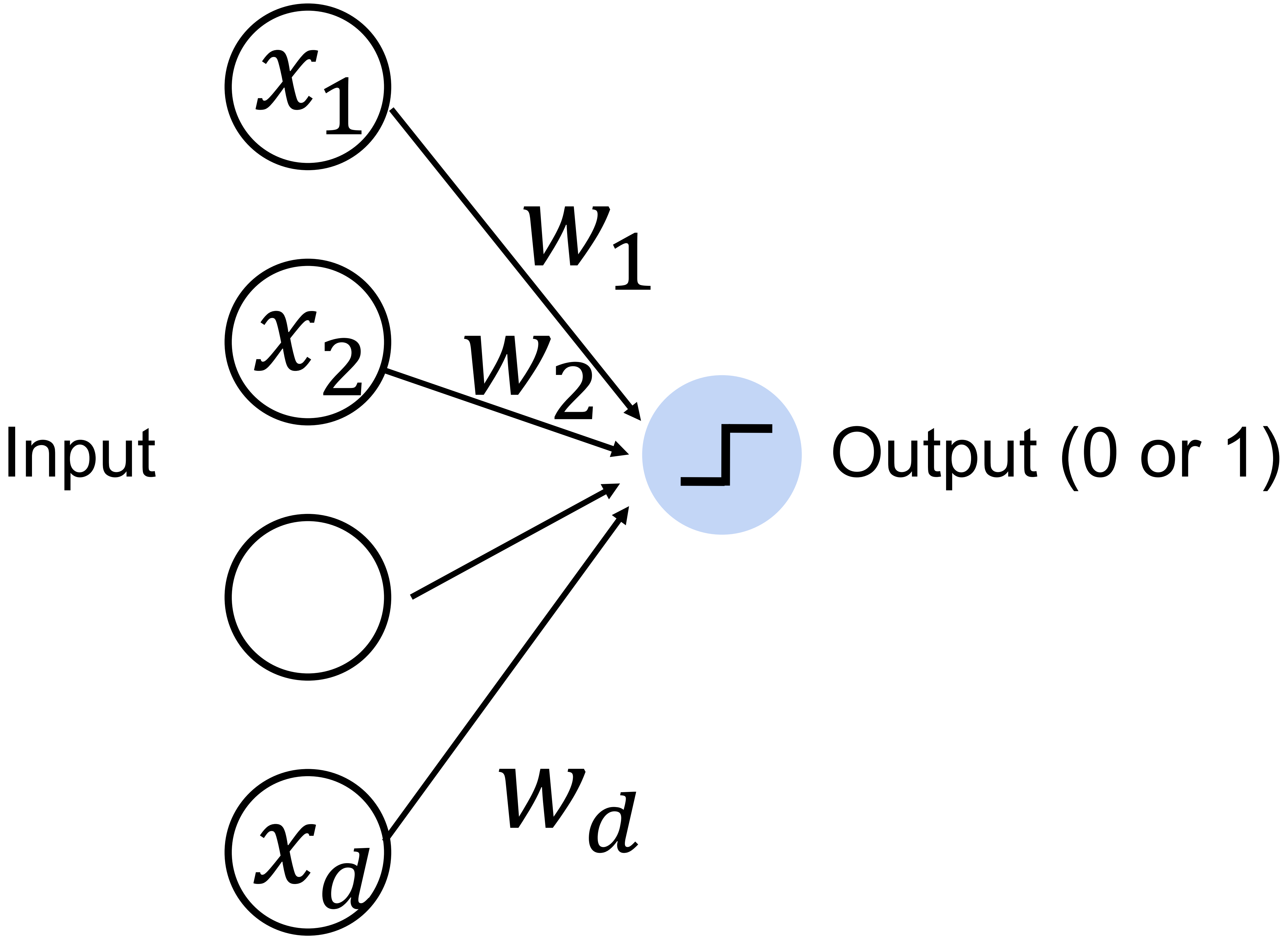
Perceptron

- Given input $\mathbf{x}$, weight $\mathbf{w}$ and bias b, perceptron outputs:

$$o = \sigma(\mathbf{w}^\top \mathbf{x} + b) \qquad \sigma(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{otherwise} \end{cases}$$

Activation function

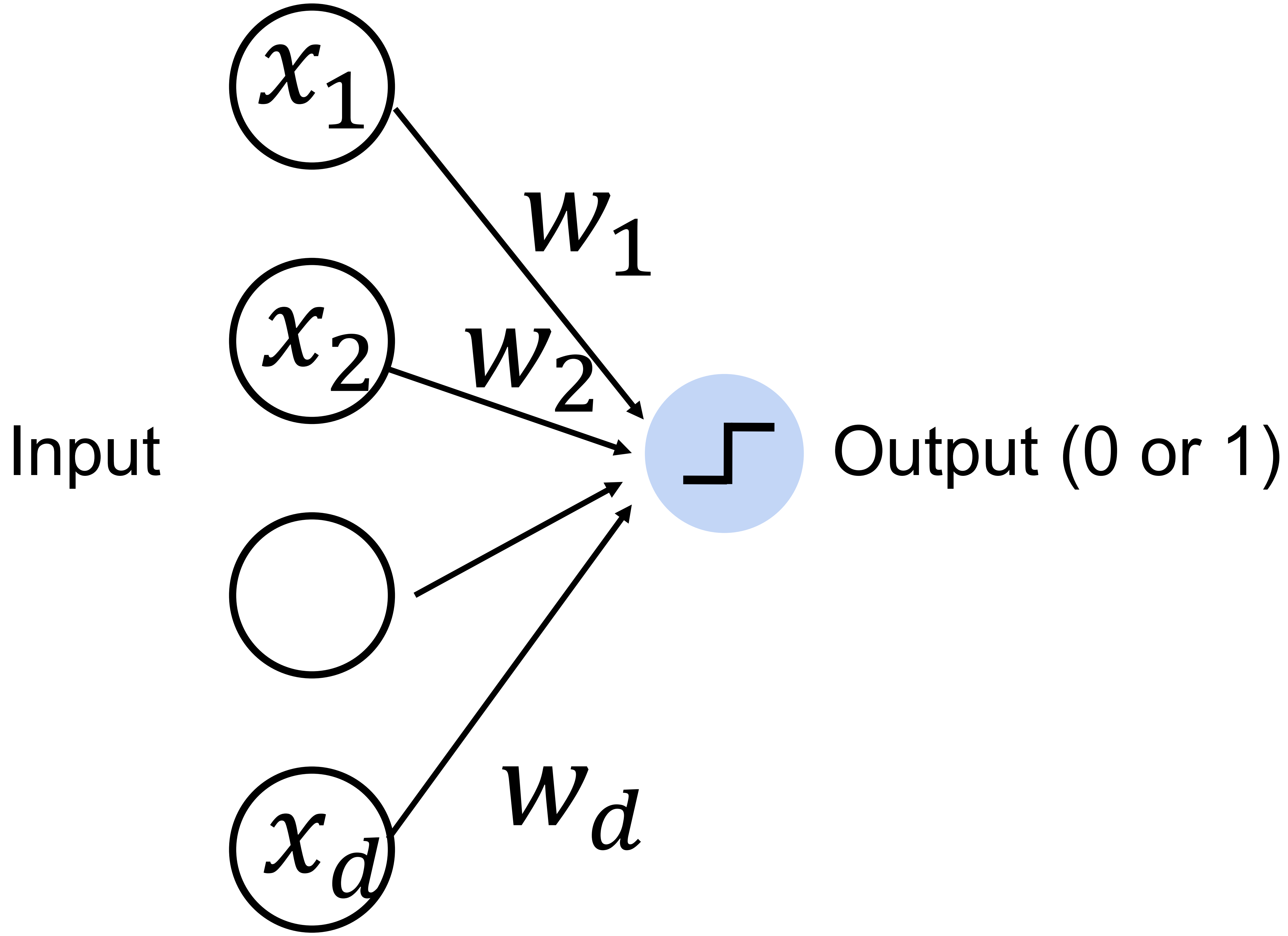
Cats vs. dogs?



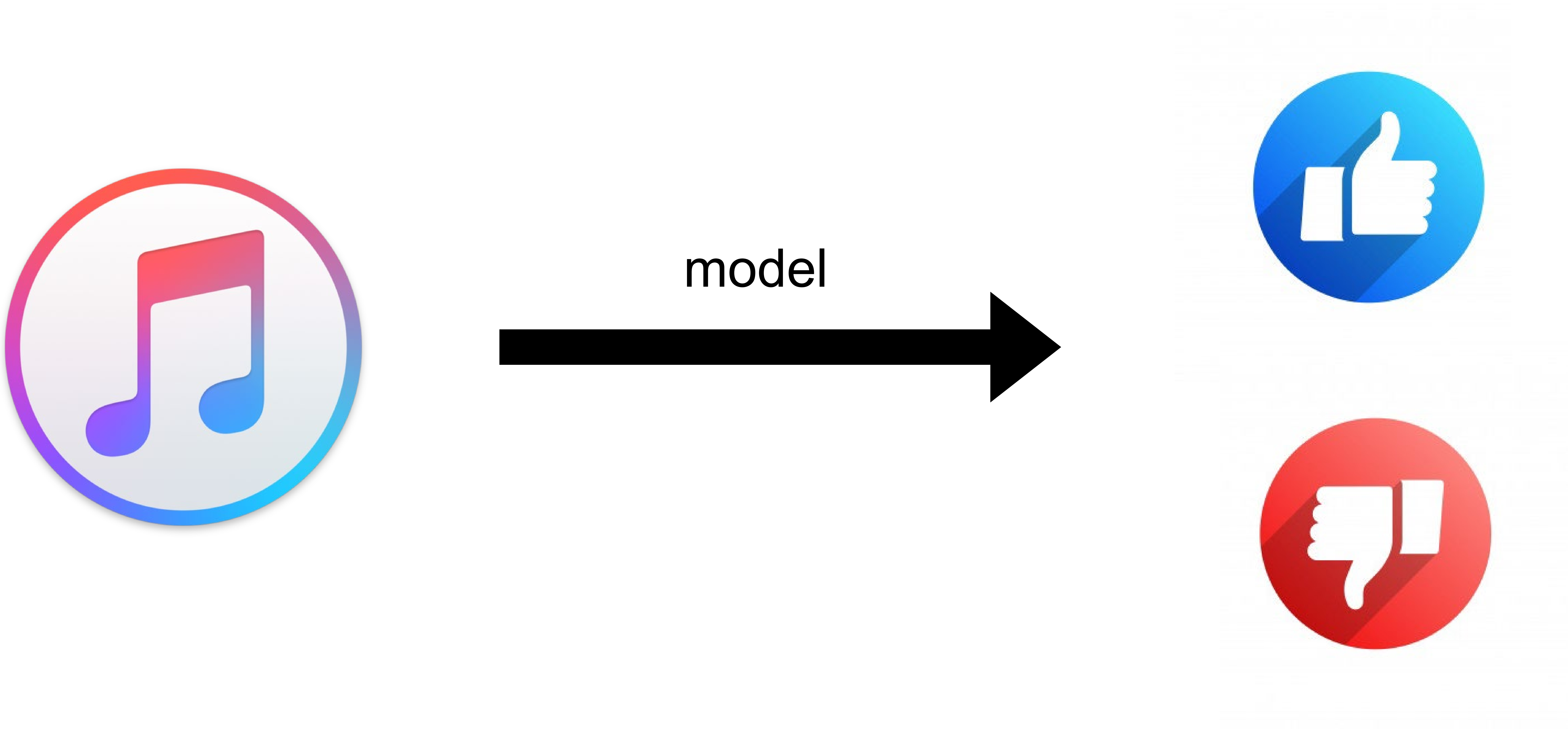
Perceptron

- Goal: learn parameters $\mathbf{w} = \{w_1, w_2, \ldots, w_d\}$ and b to minimize the classification error

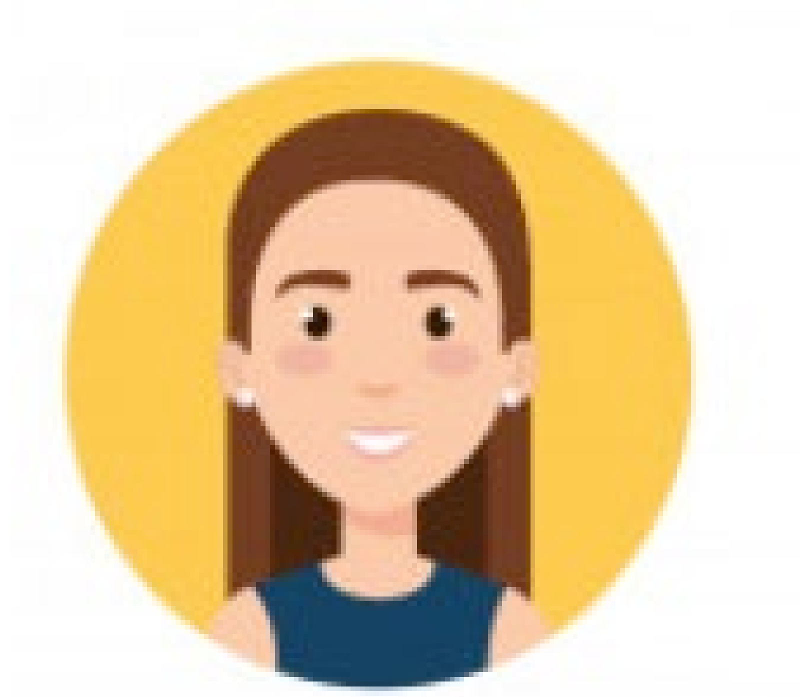
Cats vs. dogs?



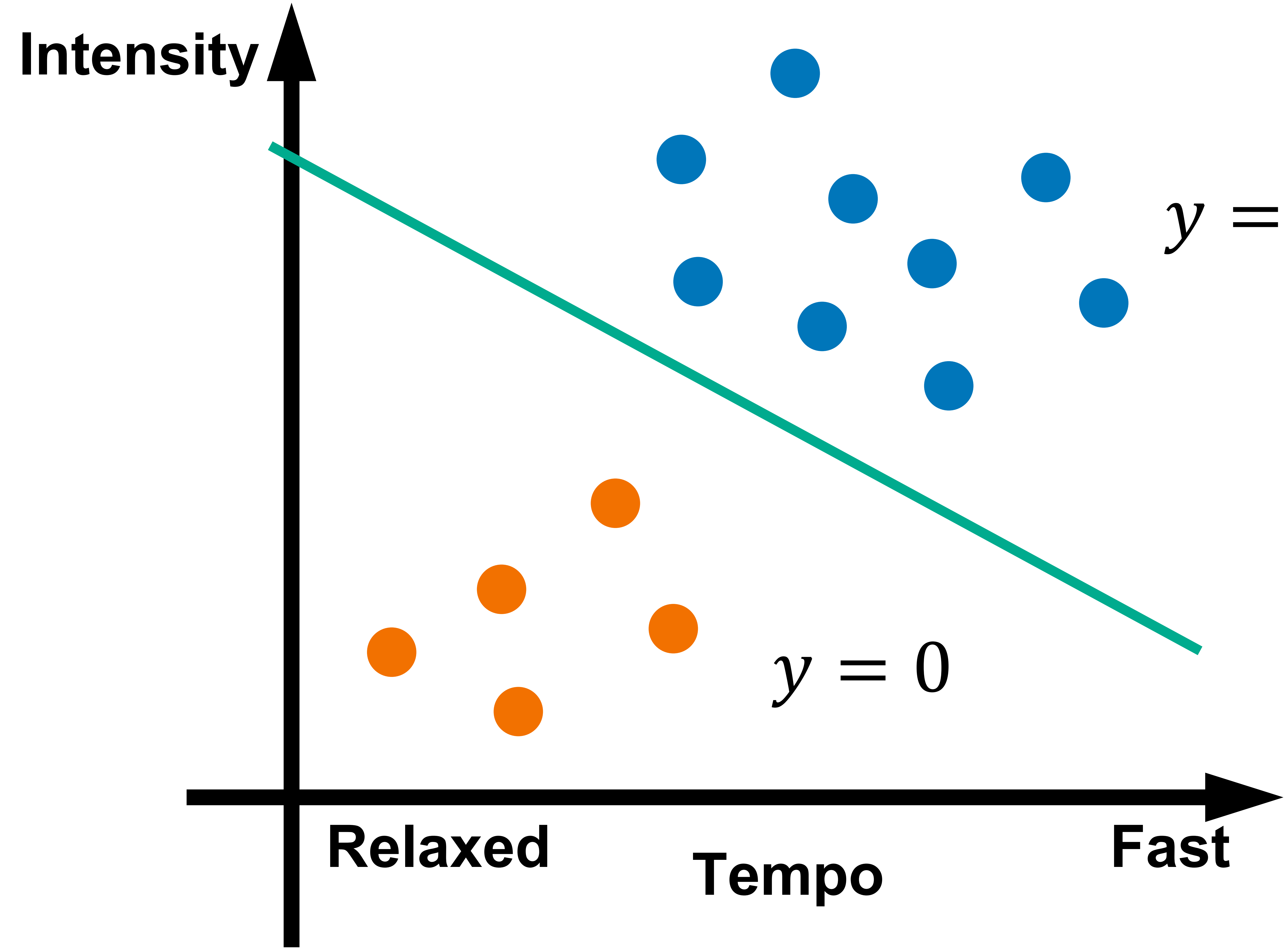
Example 2: Predict whether a user likes a song or not



Example 2: Predict whether a user likes a song or not using Perceptron



User Sharon



DisLike

Like

Learning logic functions using perceptron

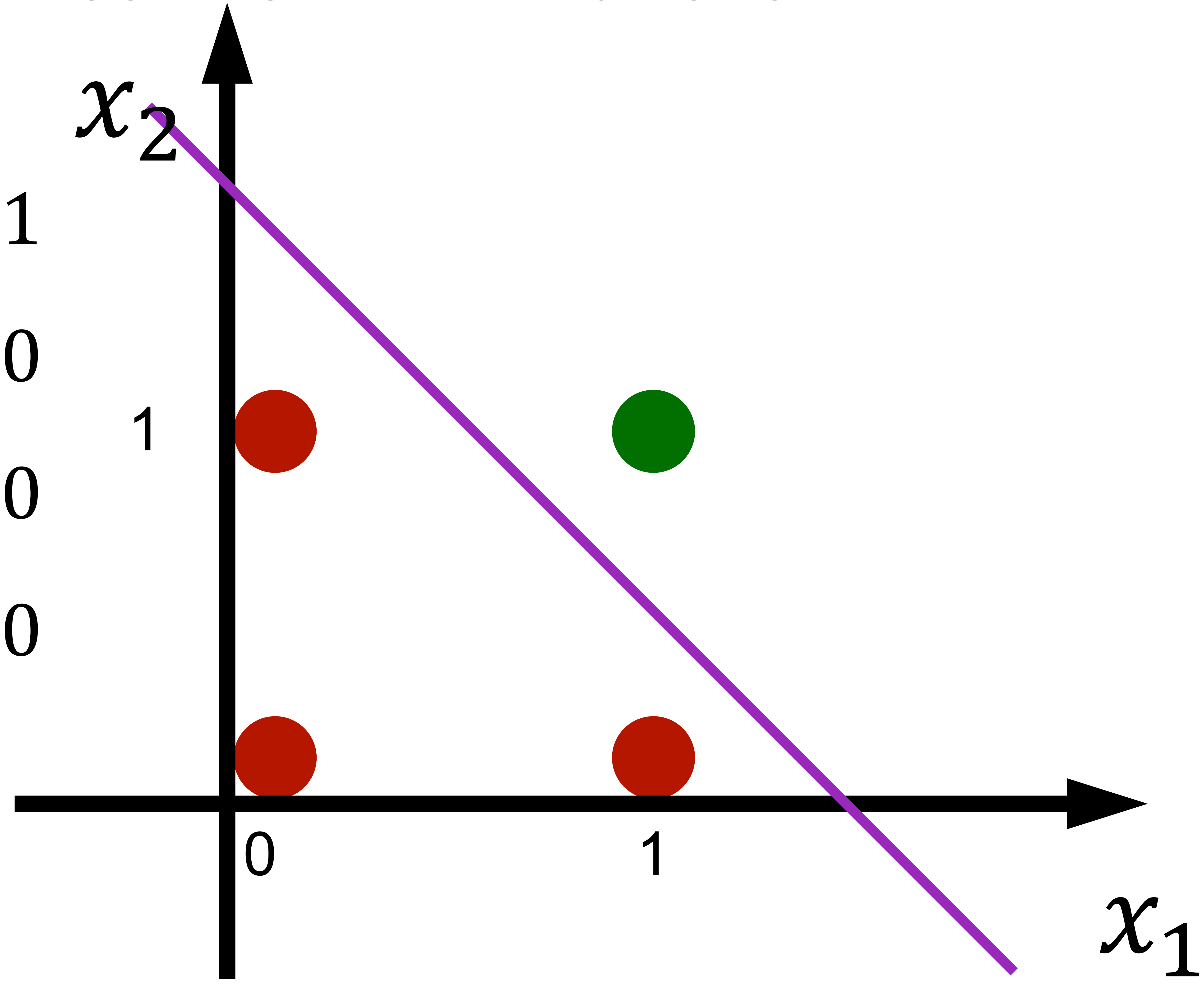
The perceptron can learn an AND function

$x_1 = 1, x_2 = 1, y = 1$

$x_1 = 1, x_2 = 0, y = 0$

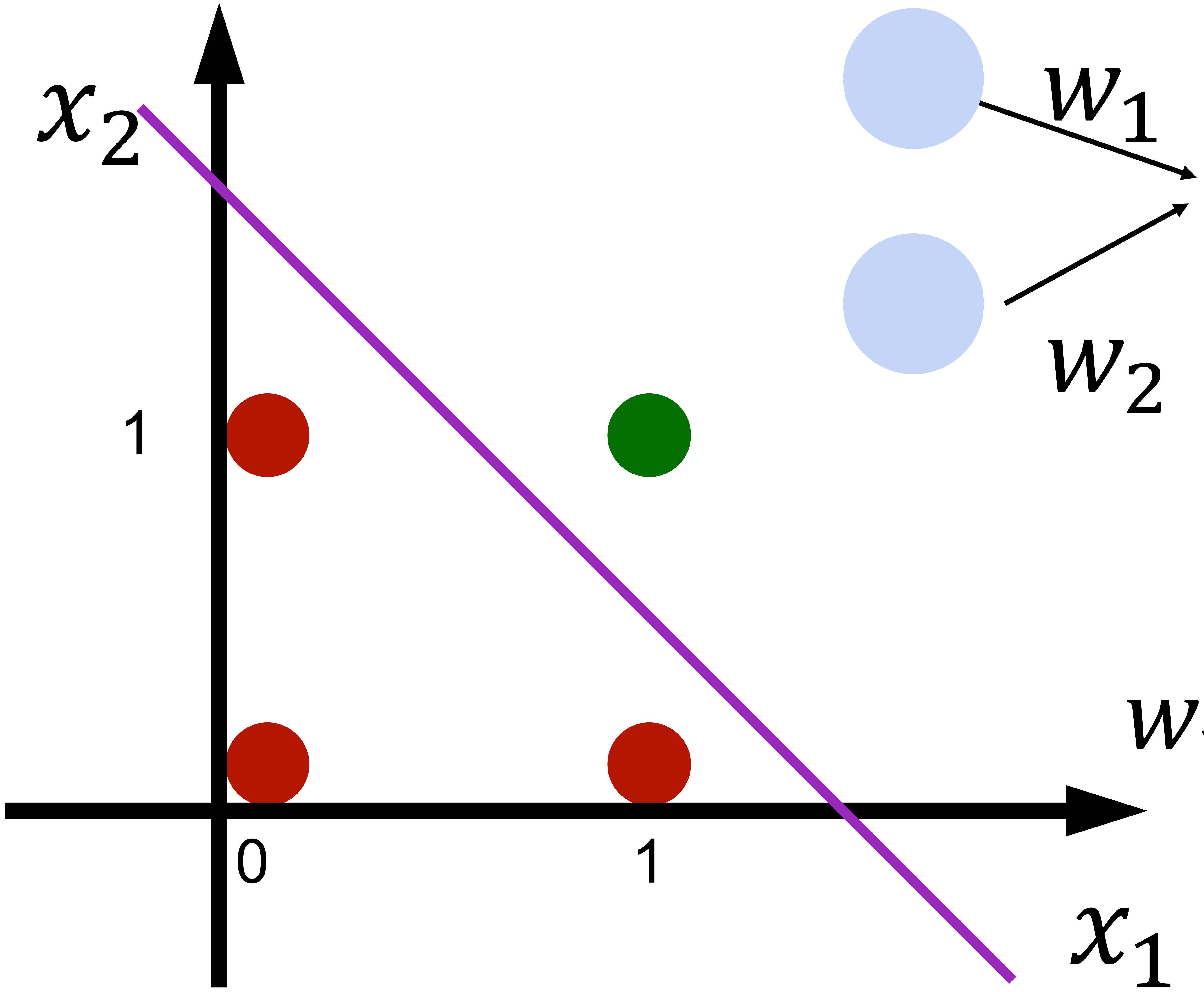
$x_1 = 0, x_2 = 1, y = 0$

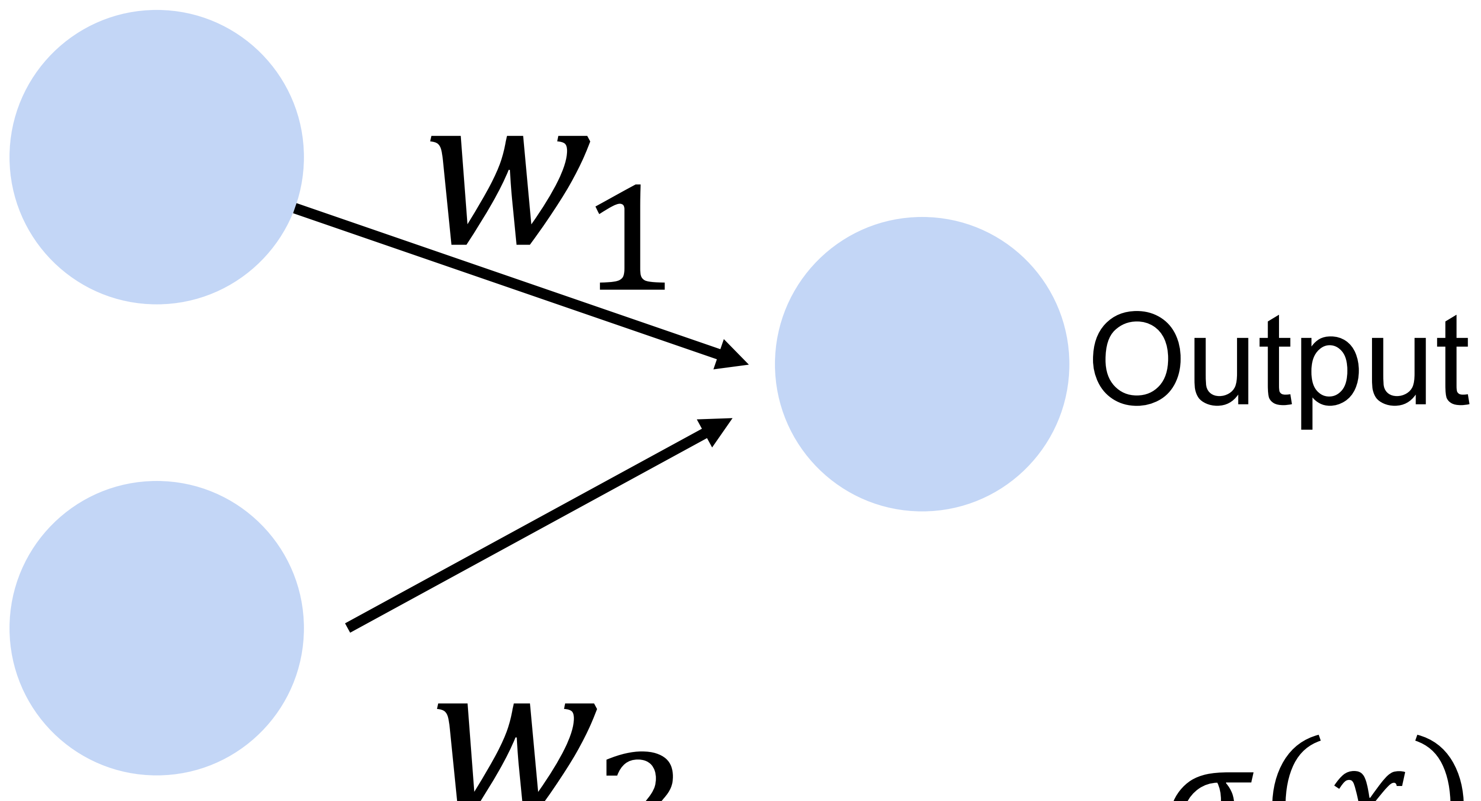
$x_1 = 0, x_2 = 0, y = 0$



Learning logic functions using perceptron

The perceptron can learn an AND function





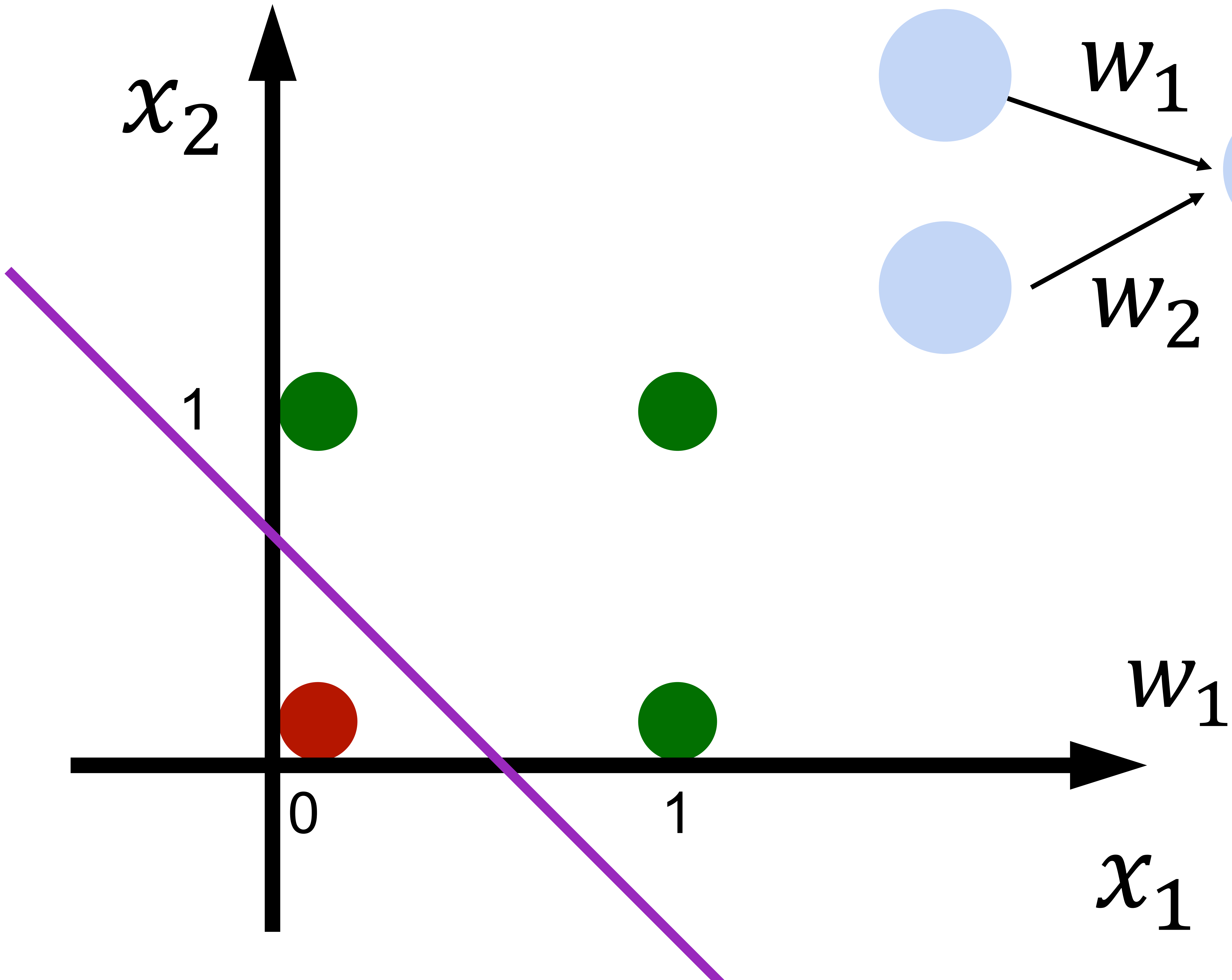
$\sigma(x_1 w_1 + x_2 w_2 + b)$

$$\sigma(x) = \begin{cases} 1 & if \;\; x > 0 \\ 0 & otherwise \end{cases}$$

$$w_1 = 1, w_2 = 1, b = -1.5$$

Learning OR function using perceptron

The perceptron can learn an OR function



Output $\sigma(x_1 w_1 + x_2 w_2 + b)$

$$\sigma(x) = \begin{cases} 1 & if\, x > 0 \\ 0 & otherwise \end{cases}$$

$$w_1 = 1, w_2 = 1, b = -0.5$$

XOR Problem (Minsky & Papert, 1969)

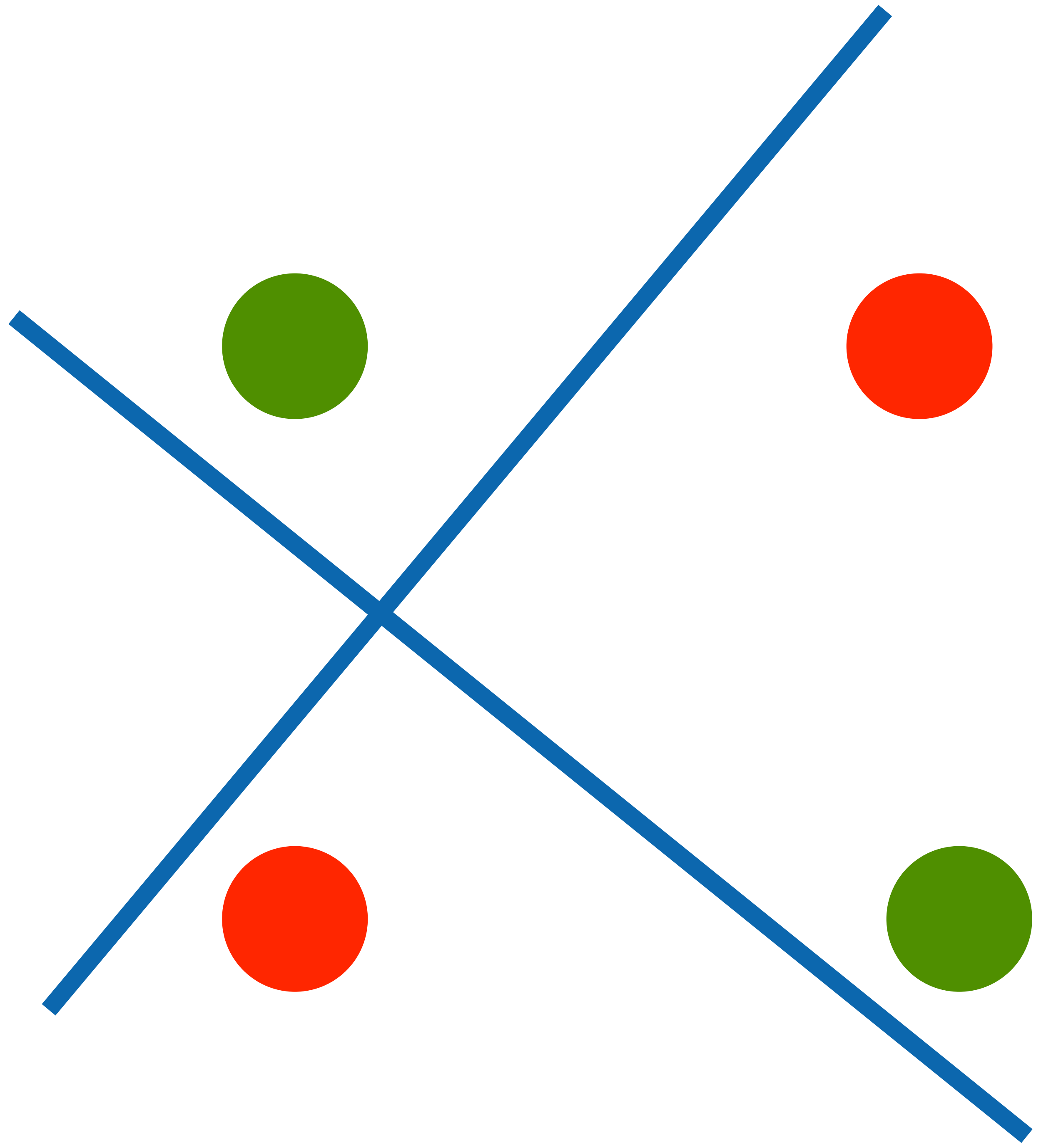
The perceptron cannot learn an XOR function
(neurons can only generate linear separators)

$x_1 = 1, x_2 = 1, y = 0$

$x_1 = 1, x_2 = 0, y = 1$

$x_1 = 0, x_2 = 1, y = 1$

$x_1 = 0, x_2 = 0, y = 0$



This contributed to the first AI winter

Quiz break

Which one of the following is NOT true about perceptron?

A. Perceptron only works if the data is linearly separable.

B. Perceptron can learn AND function

C. Perceptron can learn XOR function

D. Perceptron is a supervised learning algorithm

Quiz break

Which one of the following is NOT true about perceptron?

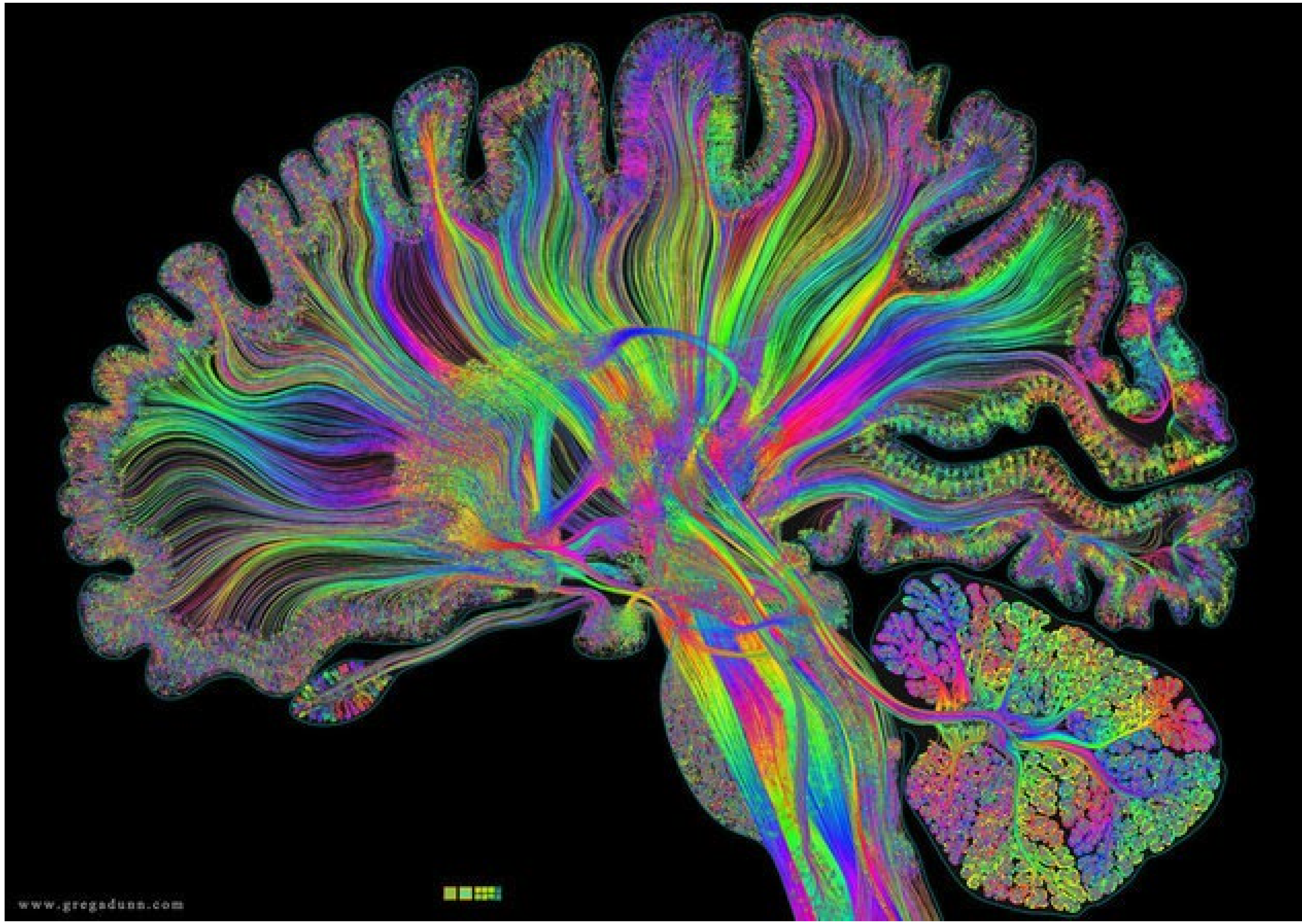
A. Perceptron only works if the data is linearly separable.

B. Perceptron can learn AND function

C. Perceptron can learn XOR function

D. Perceptron is a supervised learning algorithm

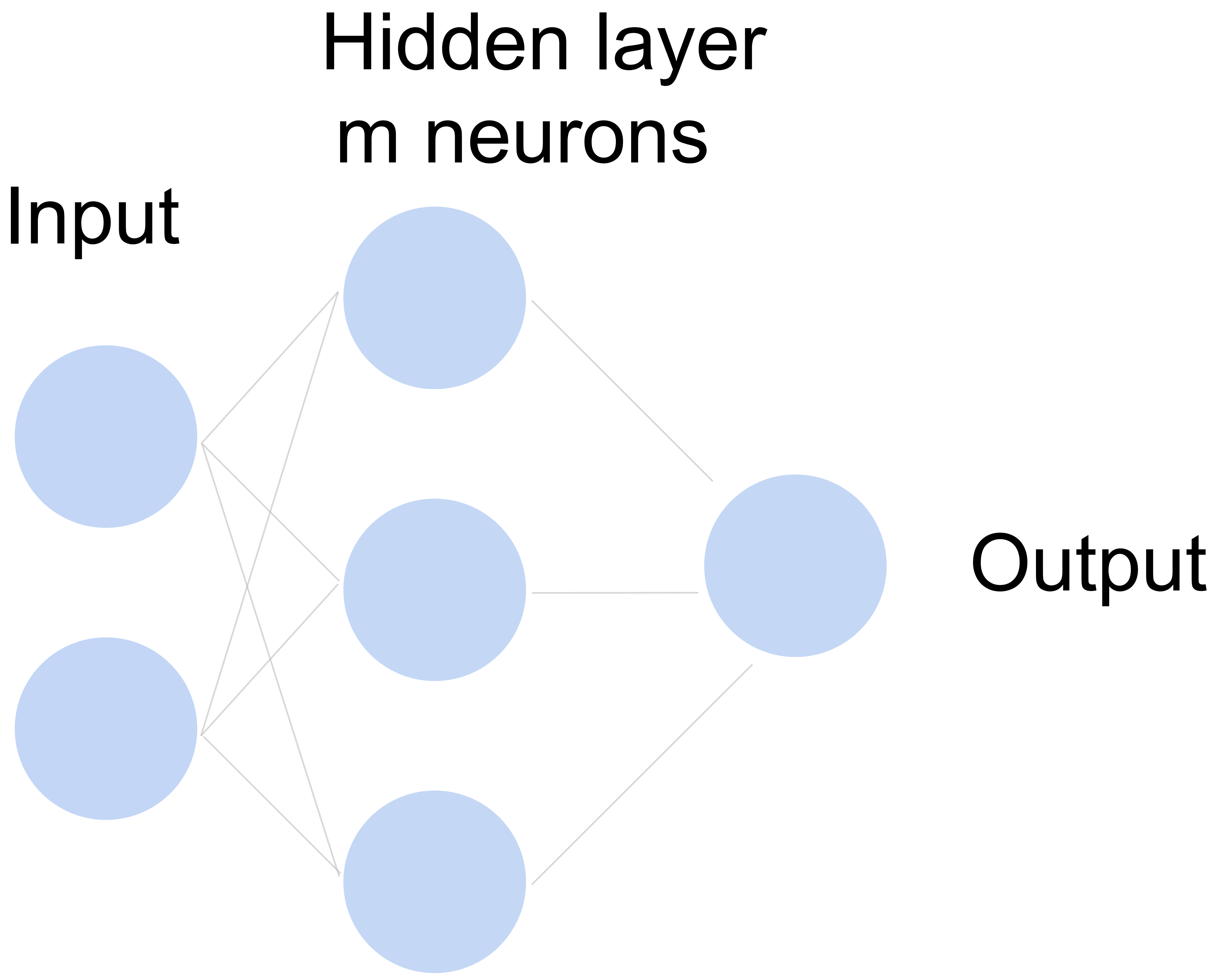
Multilayer Perceptron



Single Hidden Layer

How to classify

Cats vs. dogs?

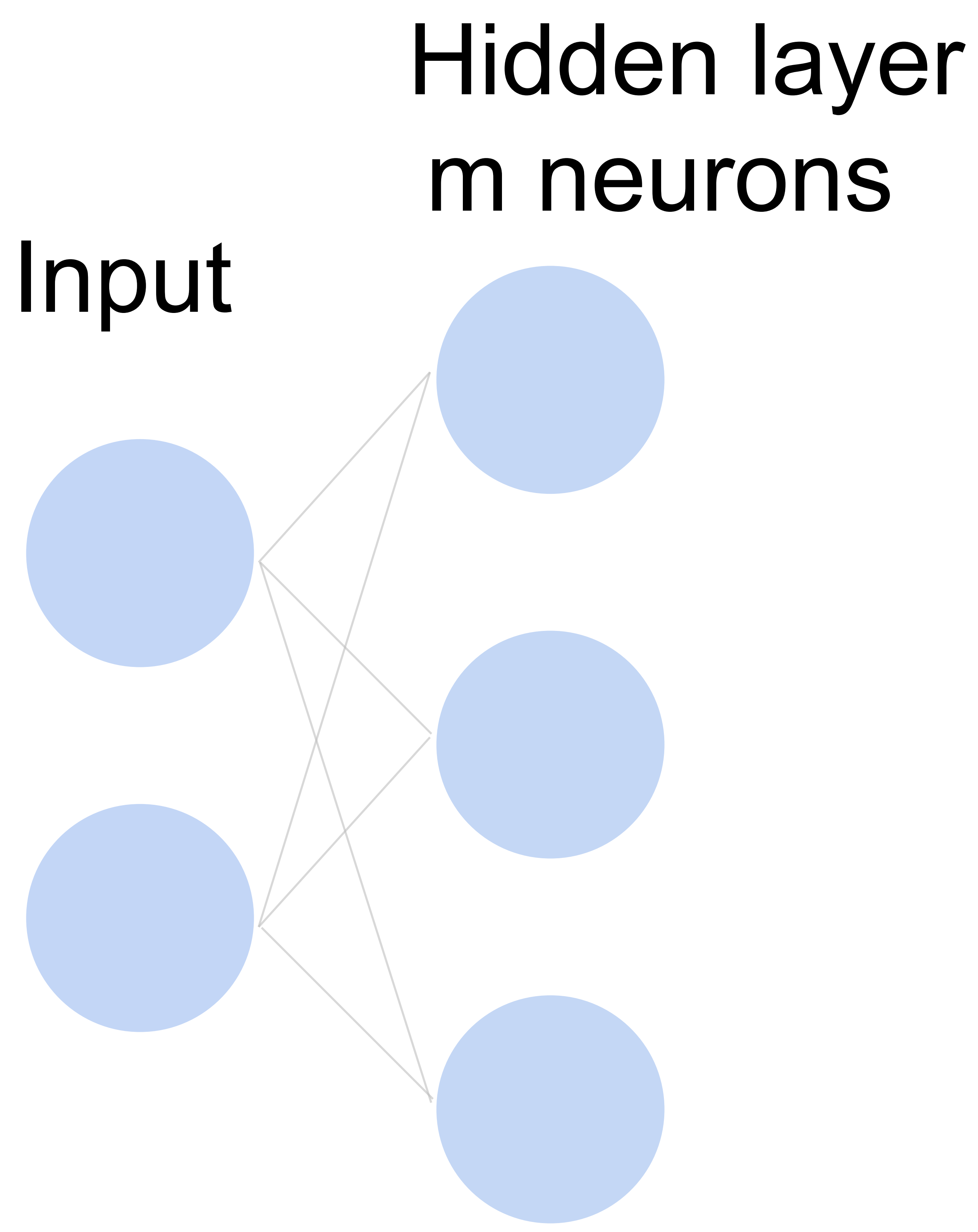


Single Hidden Layer

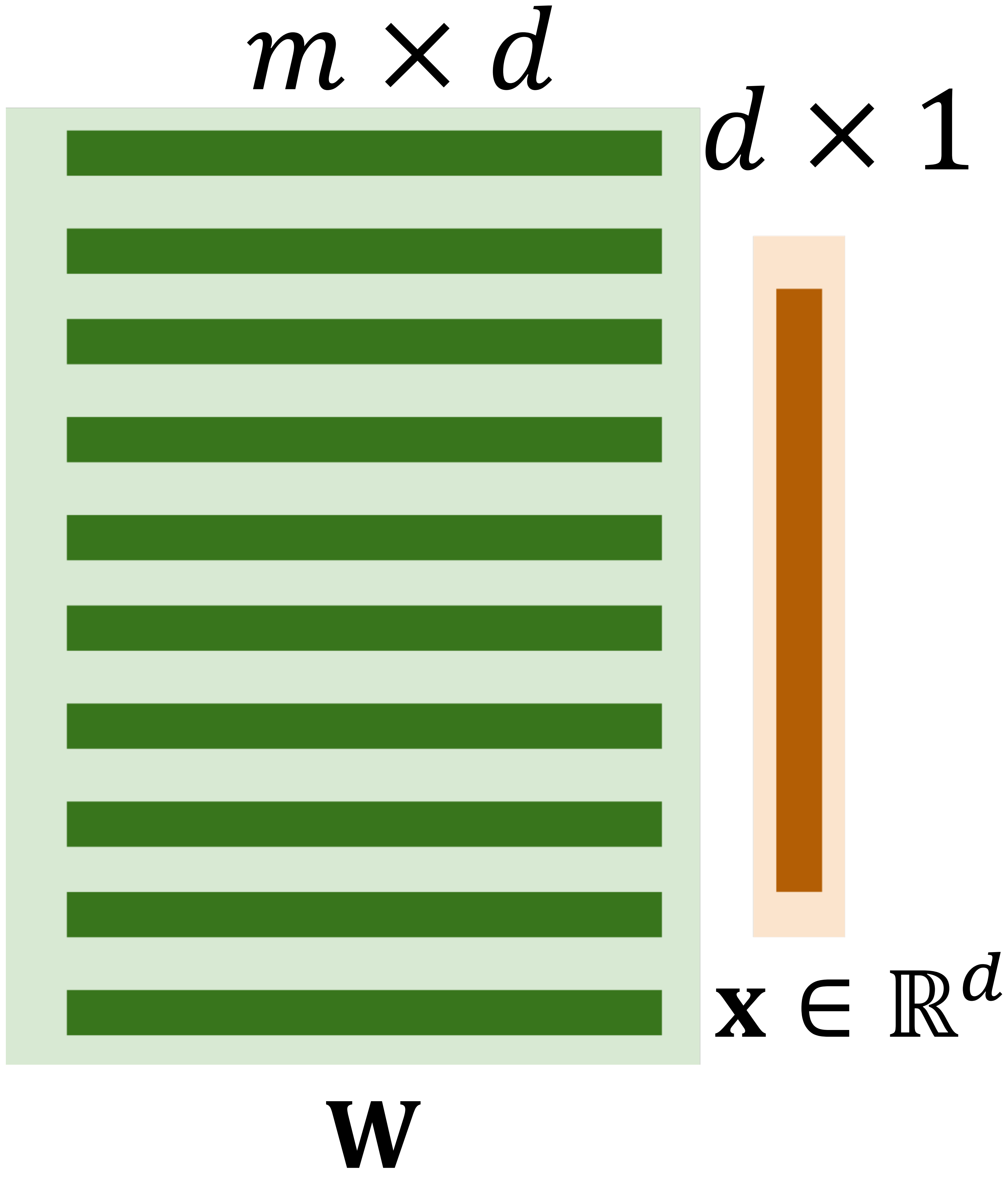
- Input $\mathbf{x} \in \mathbb{R}^d$
- Hidden $\mathbf{W} \in \mathbb{R}^{m \times d}, \mathbf{b} \in \mathbb{R}^m$
- Intermediate output

$$\mathbf{h} \quad = \sigma(\mathbf{W}\mathbf{x} + \mathbf{b})$$

σ is an element-wise activation function

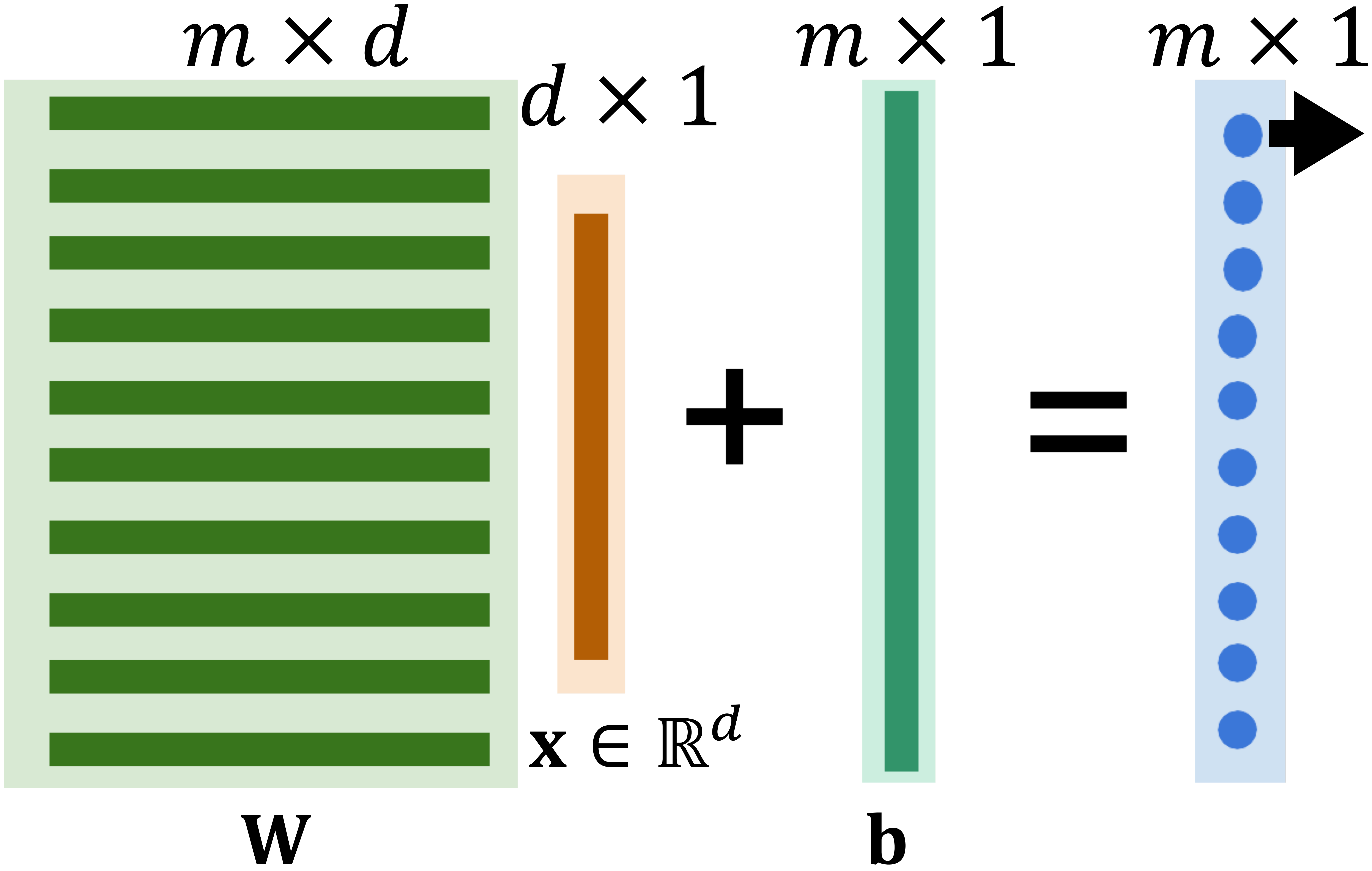


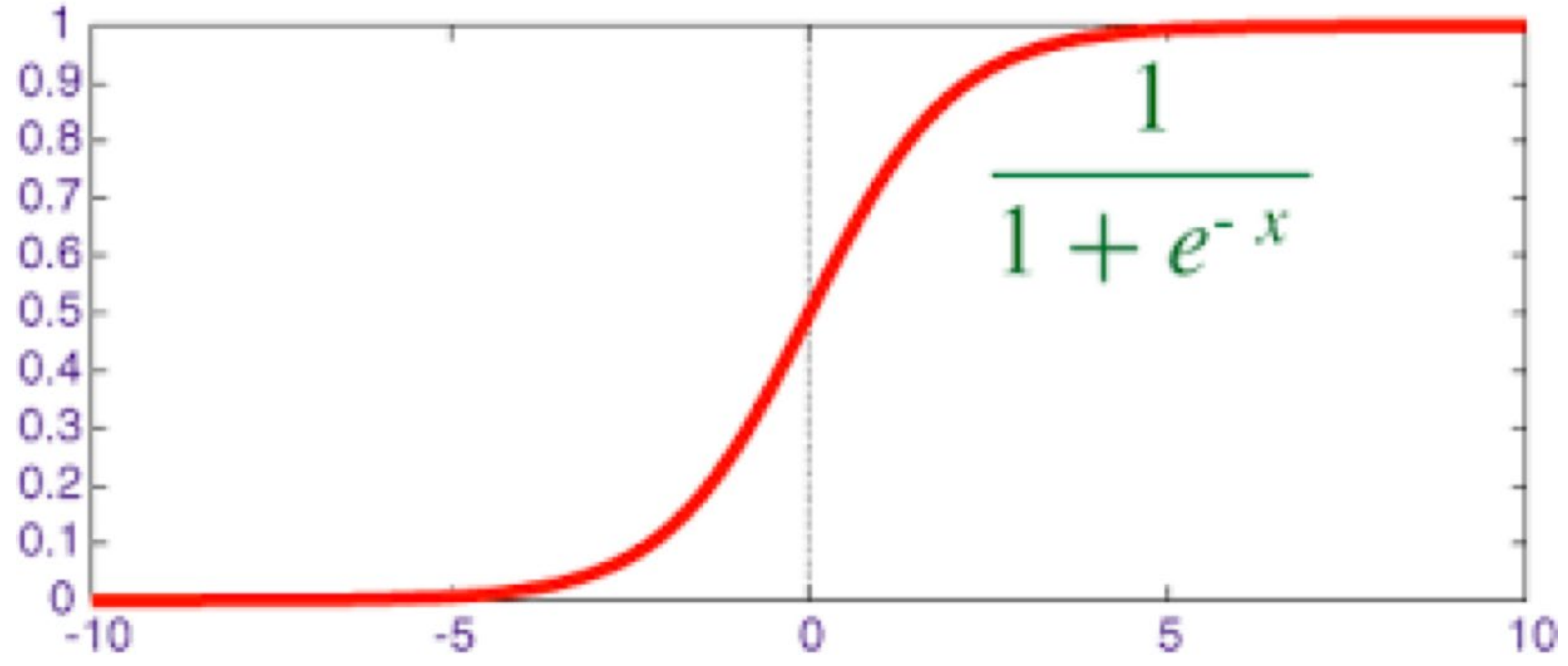
Neural networks with one hidden layer



Neural networks with one hidden layer

Key elements: linear operations + Nonlinear activations





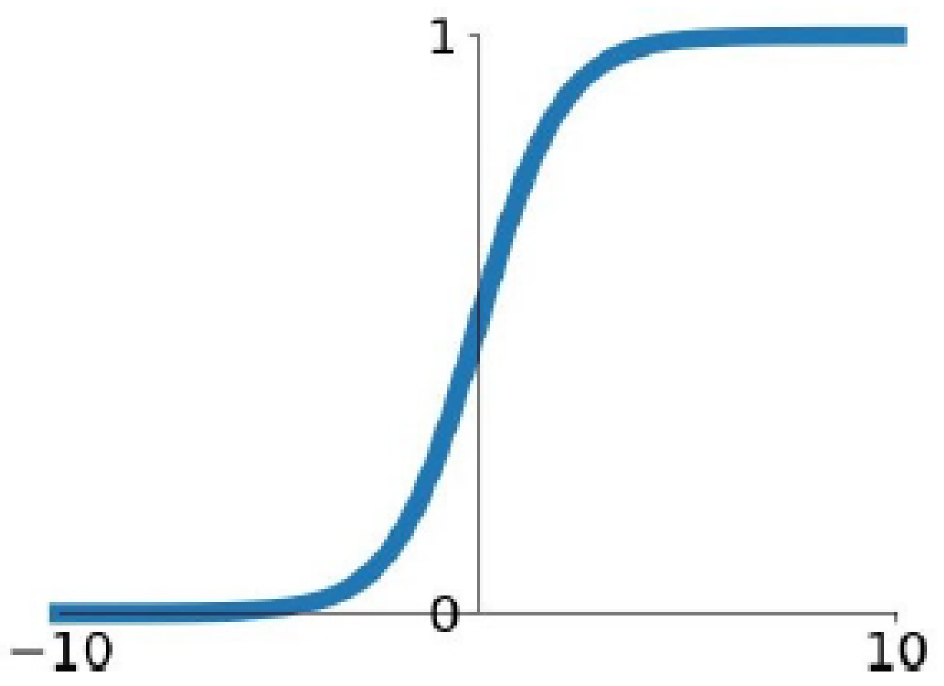
Element-wise
activation function

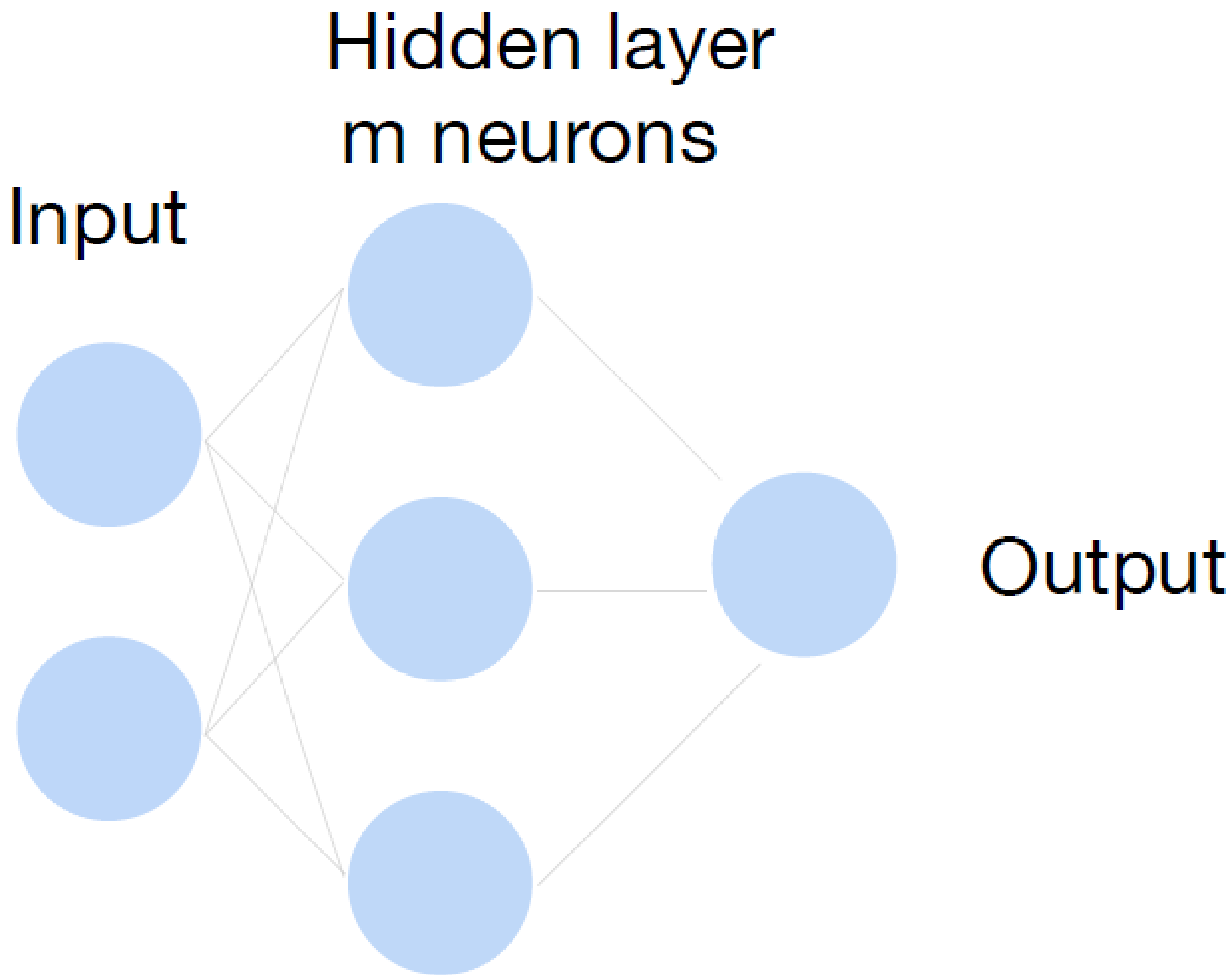
Single Hidden Layer

- Output $f = \mathbf{w}_2^\top \mathbf{h} + b_2$
- Normalize the output into probability using sigmoid

$$p(y = 1 \mid \mathbf{x}) = \frac{1}{1 + e^{-f}}$$

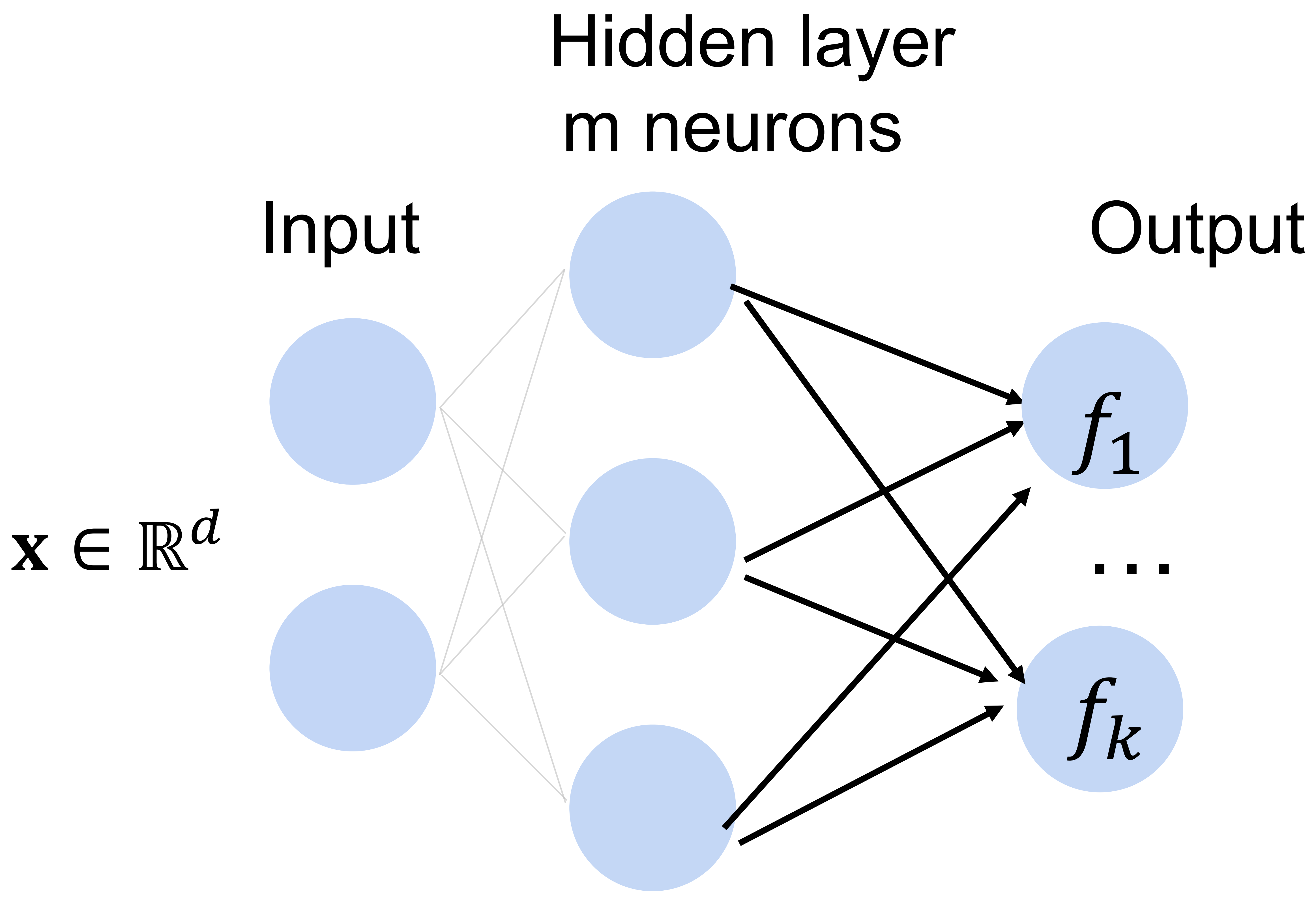
Sigmoid





Multi-class classification

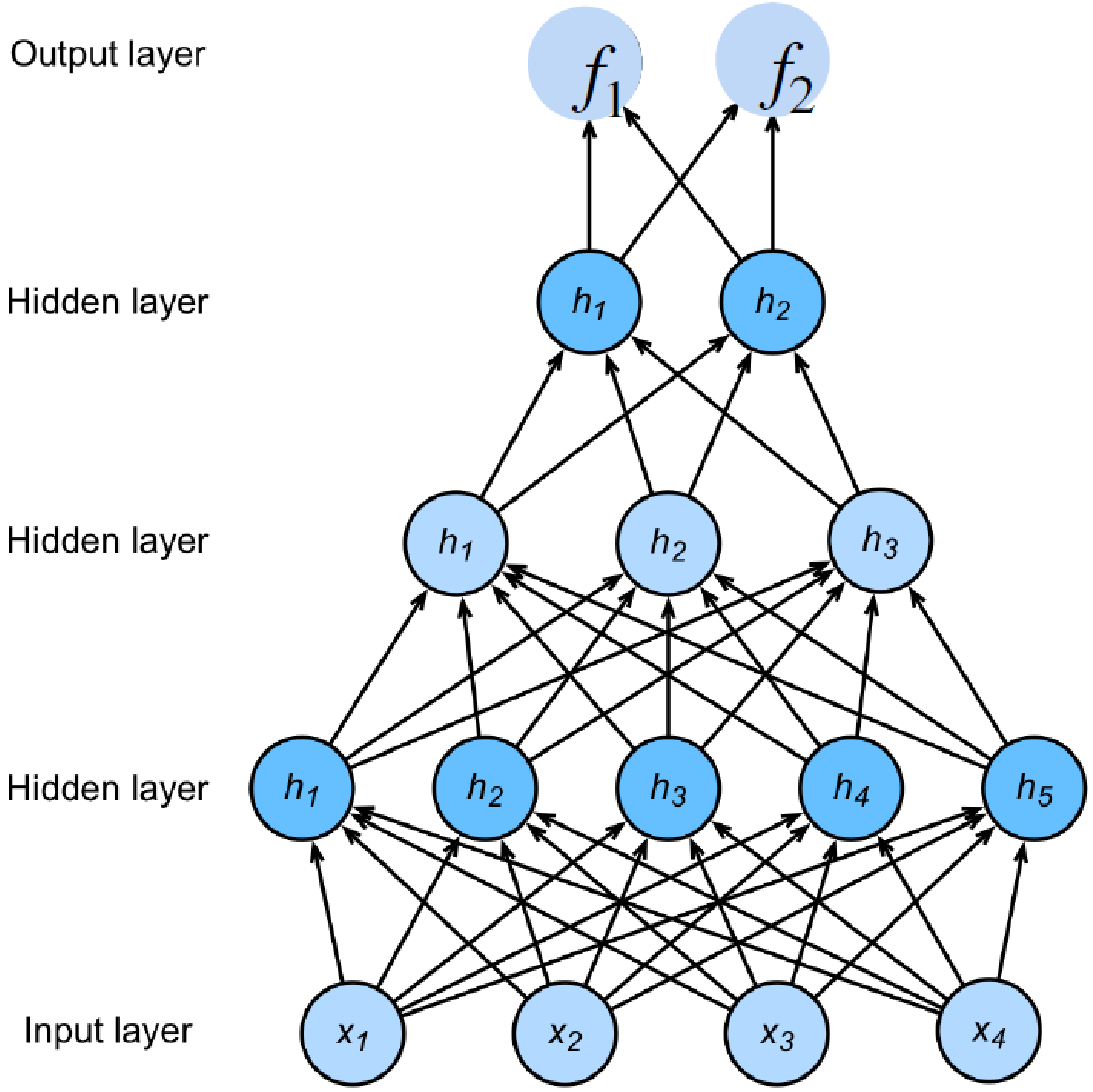
Turns outputs *f* into *k* probabilities (sum up to 1 across *k* classes)



$$p(y|\mathbf{x}) = softmax(\mathbf{f})$$

$$= \frac{\exp f_y(x)}{\sum_i^k \exp f_i(x)}$$

Deep neural networks (DNNs)



$$\mathbf{h}_1 = \sigma(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1)$$

$$\mathbf{h}_2 = \sigma(\mathbf{W}_2\mathbf{h}_1 + \mathbf{b}_2)$$

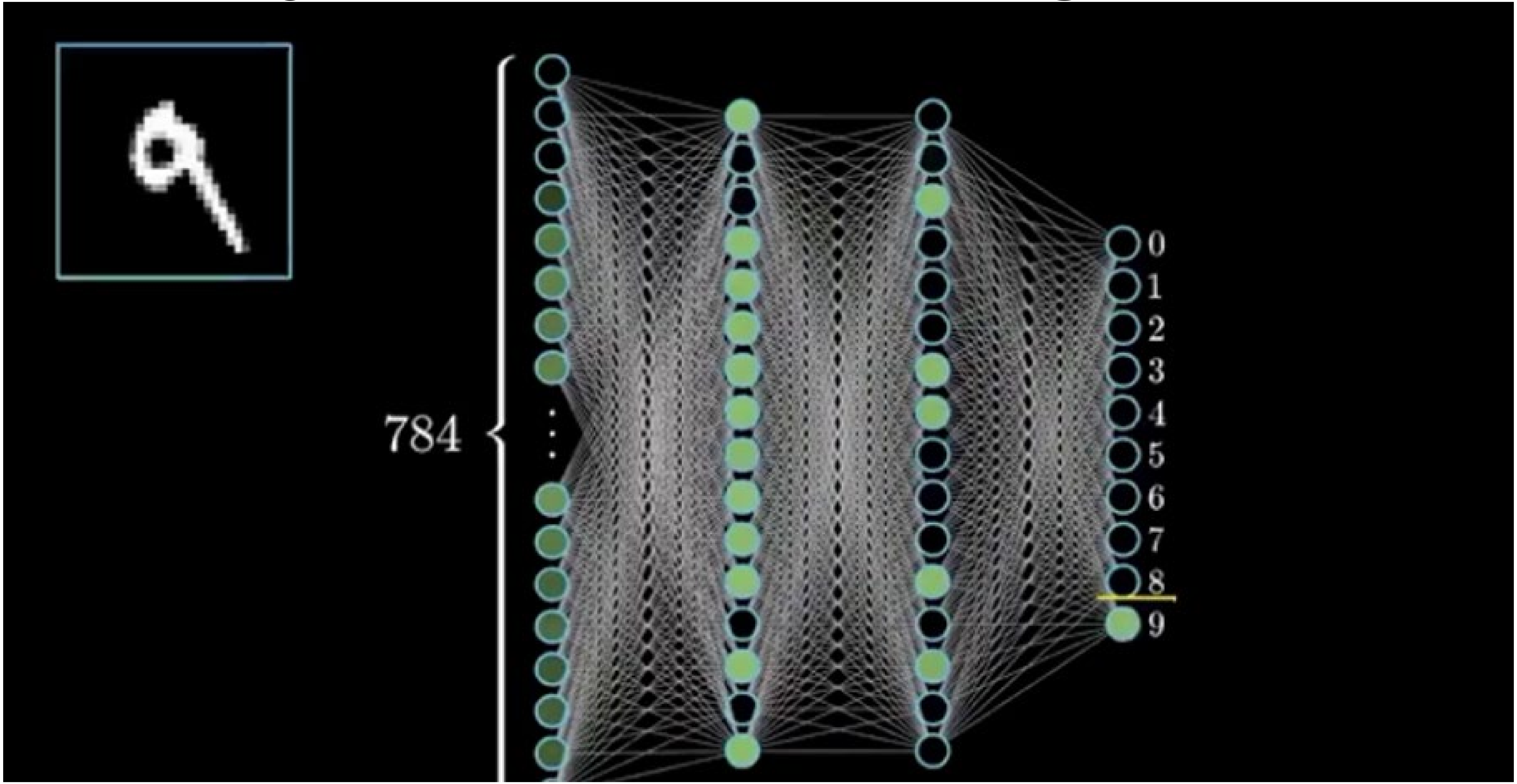
$$\mathbf{h}_3 = \sigma(\mathbf{W}_3\mathbf{h}_2 + \mathbf{b}_3)$$

$$\mathbf{f} = \mathbf{W}_4\mathbf{h}_3 + \mathbf{b}_4$$

$$\mathbf{y} = \mathrm{softmax}(\mathbf{f})$$

NNs are composition of nonlinear functions

Classify MNIST handwritten digits



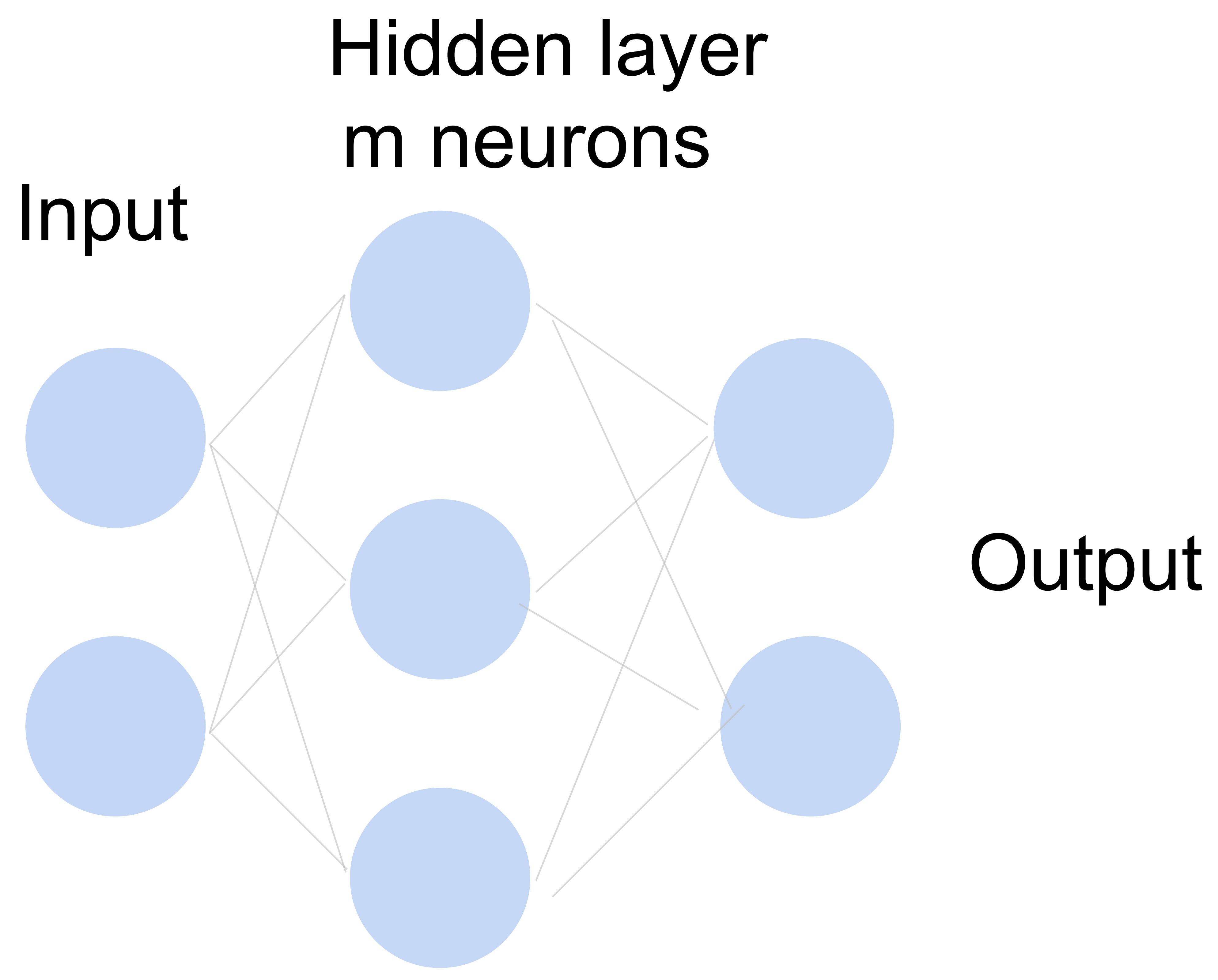
How to train a neural network?

Loss function: $$\frac{1}{|D|}\sum_i \ell(\mathbf{x}_i, y_i)$$

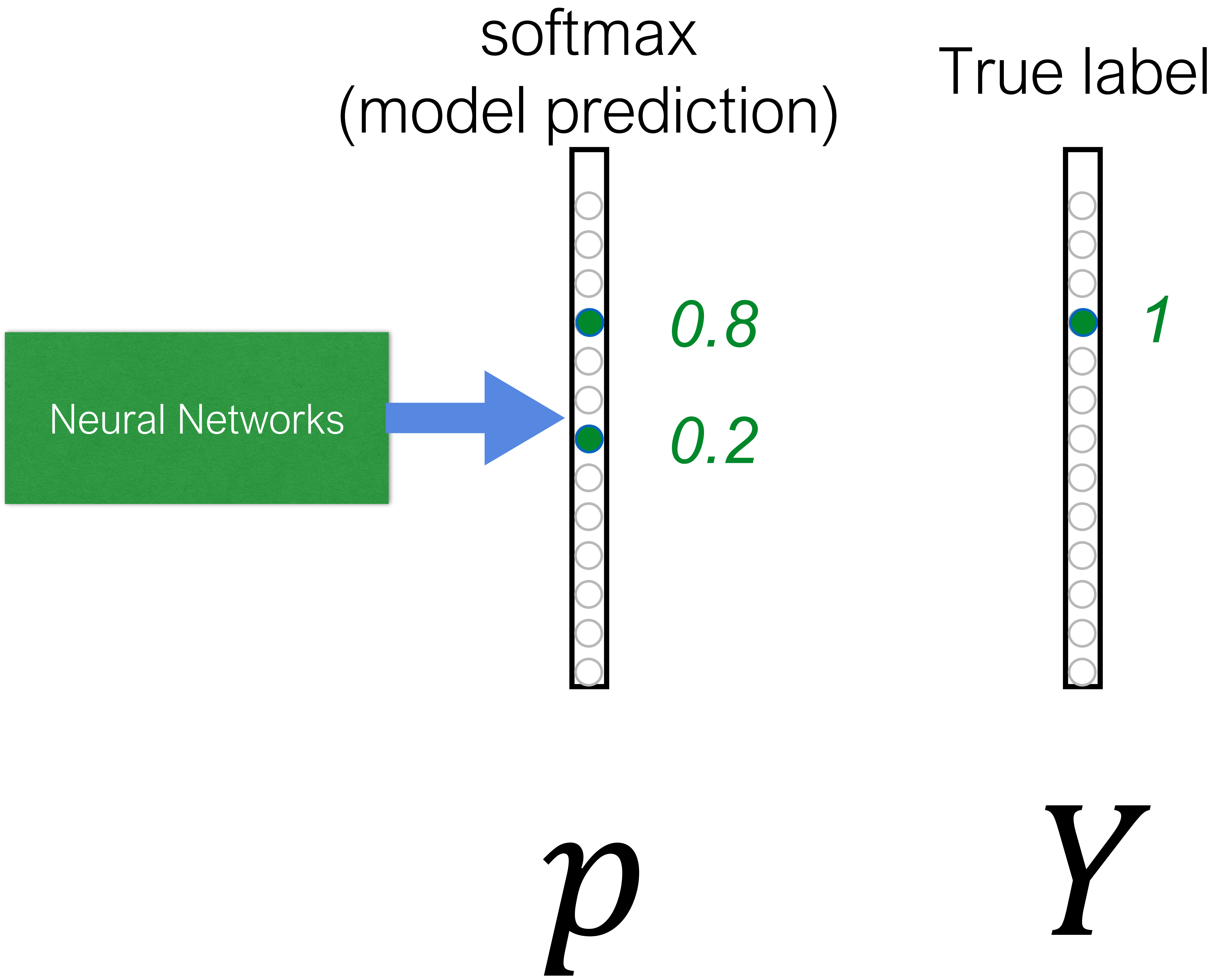
Per-sample loss:

$$\ell(\mathbf{x}, y) = \sum_{j=1}^{K} - y_j \log p_j$$

Also known as cross-entropy loss or softmax loss



Cross-Entropy Loss



$$L_{CE} = \sum_j - y_j \log(p_j)$$

$$= -\log(0.8)$$

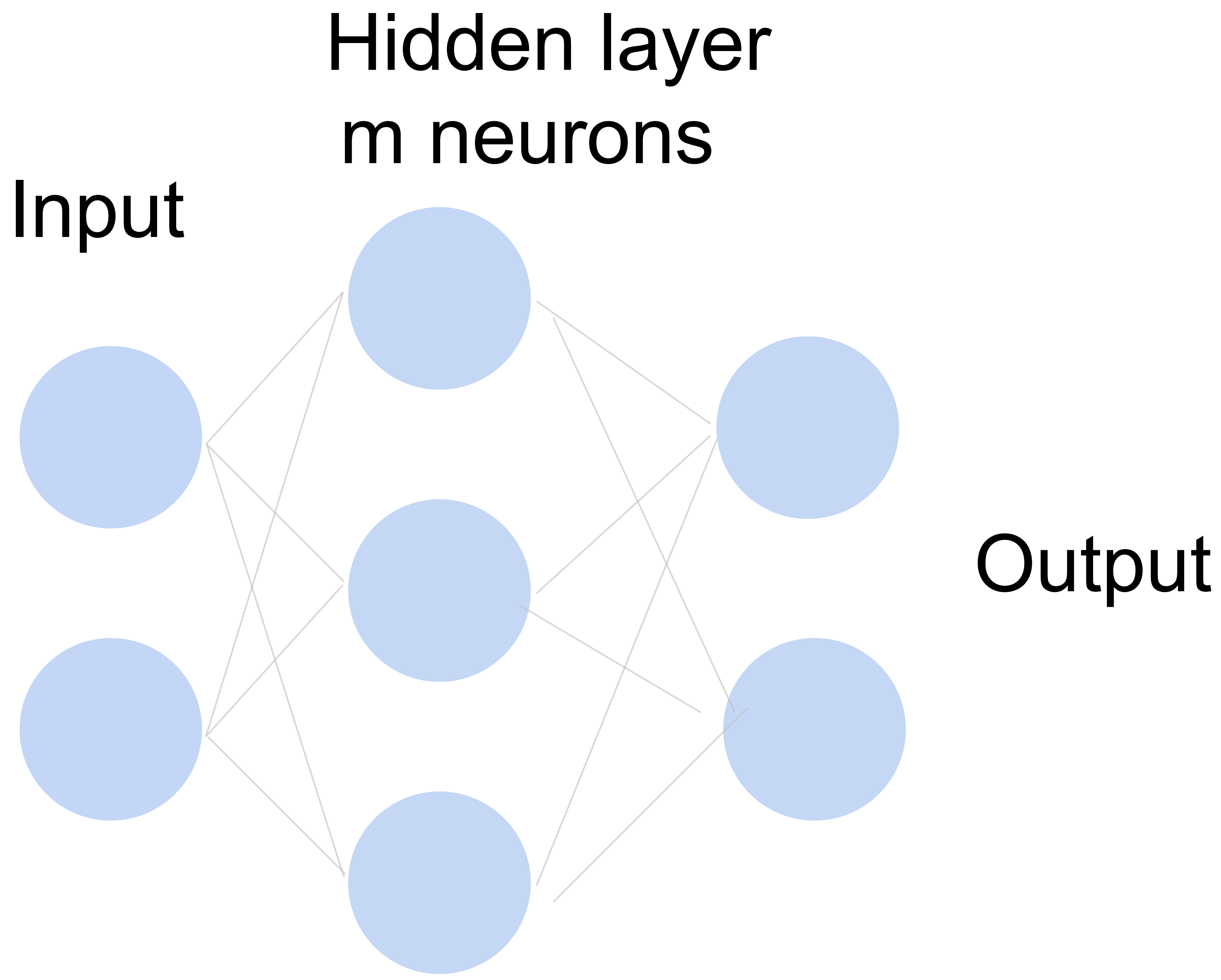
Goal: push ***p*** and ***Y*** to be identical

How to train a neural network?

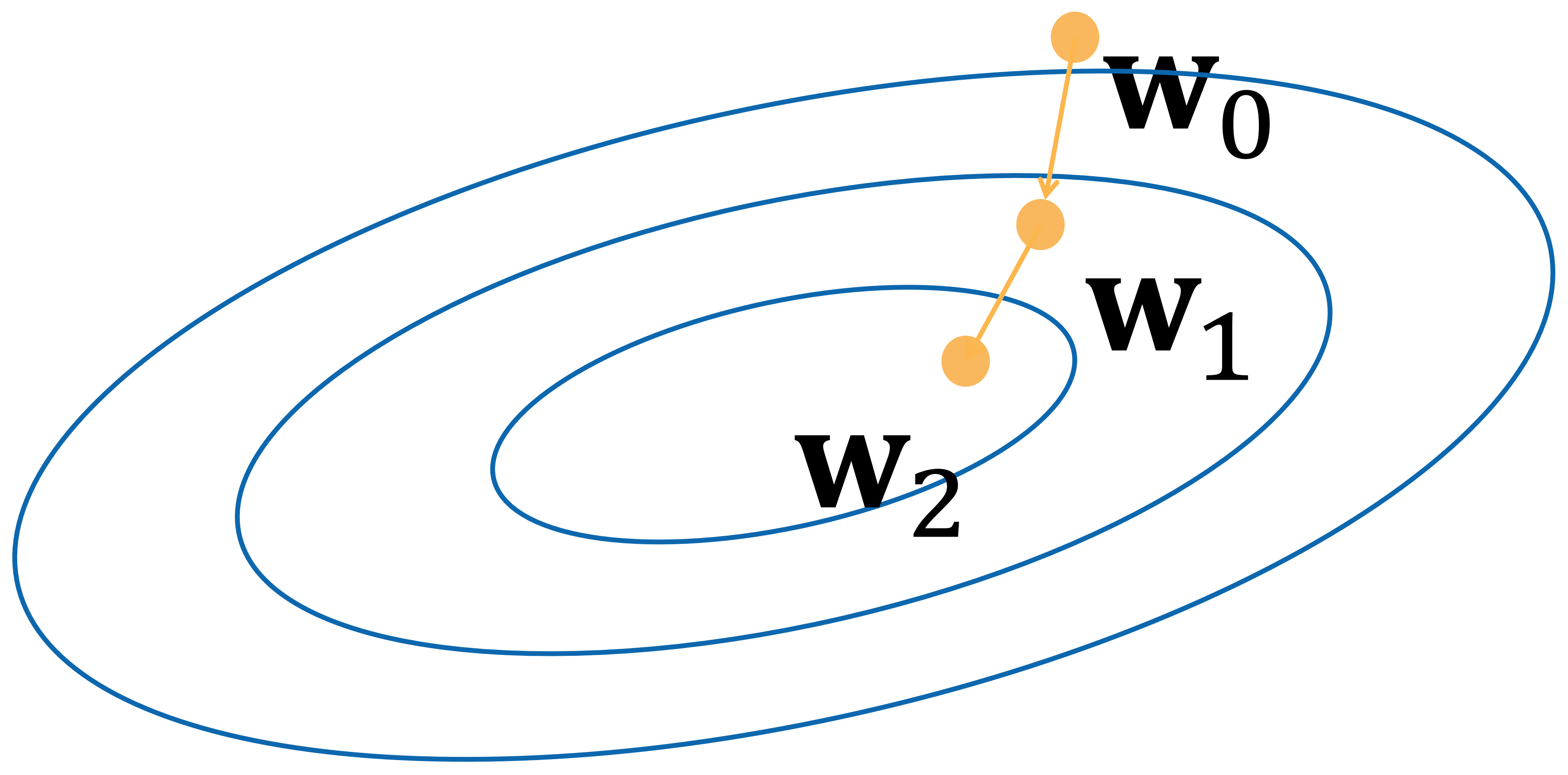
Update the weights W to minimize the loss function

$$L = \frac{1}{|D|}\sum_i \ell(\mathbf{x}_i, y_i)$$

Use gradient descent!



Gradient Descent



- Choose a learning rate $\alpha > 0$
- Initialize the model parameters w_0
- For t =1, 2, …
    - Update parameters:

$$\mathbf{w}_t = \mathbf{w}_{t-1} - \alpha \frac{\partial L}{\partial \mathbf{w}_{t-1}}$$

$$= \mathbf{w}_{t-1} - \alpha \frac{1}{|D|} \sum_{\mathbf{x} \in D} \frac{\partial \ell(\mathbf{x}_i, y_i)}{\partial \mathbf{w}_{t-1}}$$

D can be very large. Expensive per iteration

- Repeat until converges

Minibatch Stochastic Gradient Descent

- Choose a learning rate $\alpha > 0$
- Initialize the model parameters w_0
- For *t* =1, 2, …
  - **Randomly sample a subset (mini-batch)** $B \subset D$
    Update parameters:

$$\mathbf{w}_t = \mathbf{w}_{t-1} - \alpha \frac{1}{|B|} \sum_{\mathbf{x} \in B} \frac{\partial \ell(\mathbf{x}_i, y_i)}{\partial \mathbf{w}_{t-1}}$$

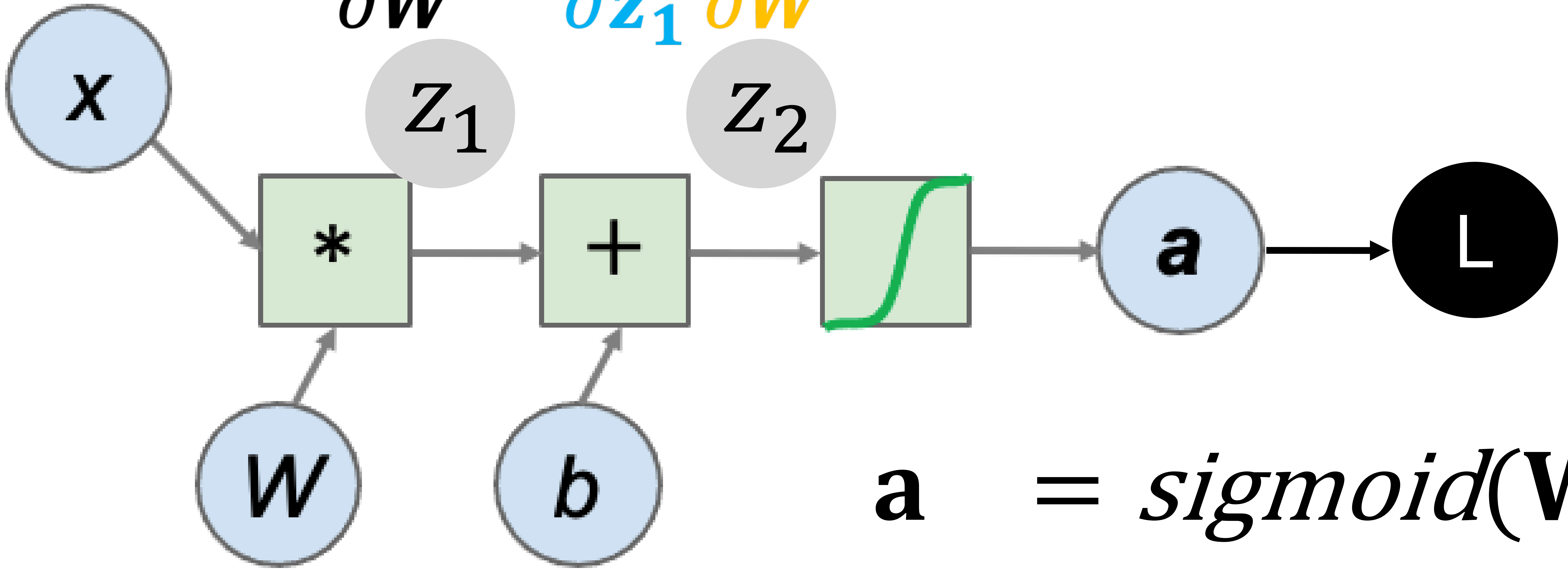
- Repeat

Calculate gradient: backpropagation with chain rule

- Define a loss function L, must compute $\frac{\partial L}{\partial \mathbf{W}}, \frac{\partial L}{\partial b}$ for all weights and biases.
- Gradient to a variable =

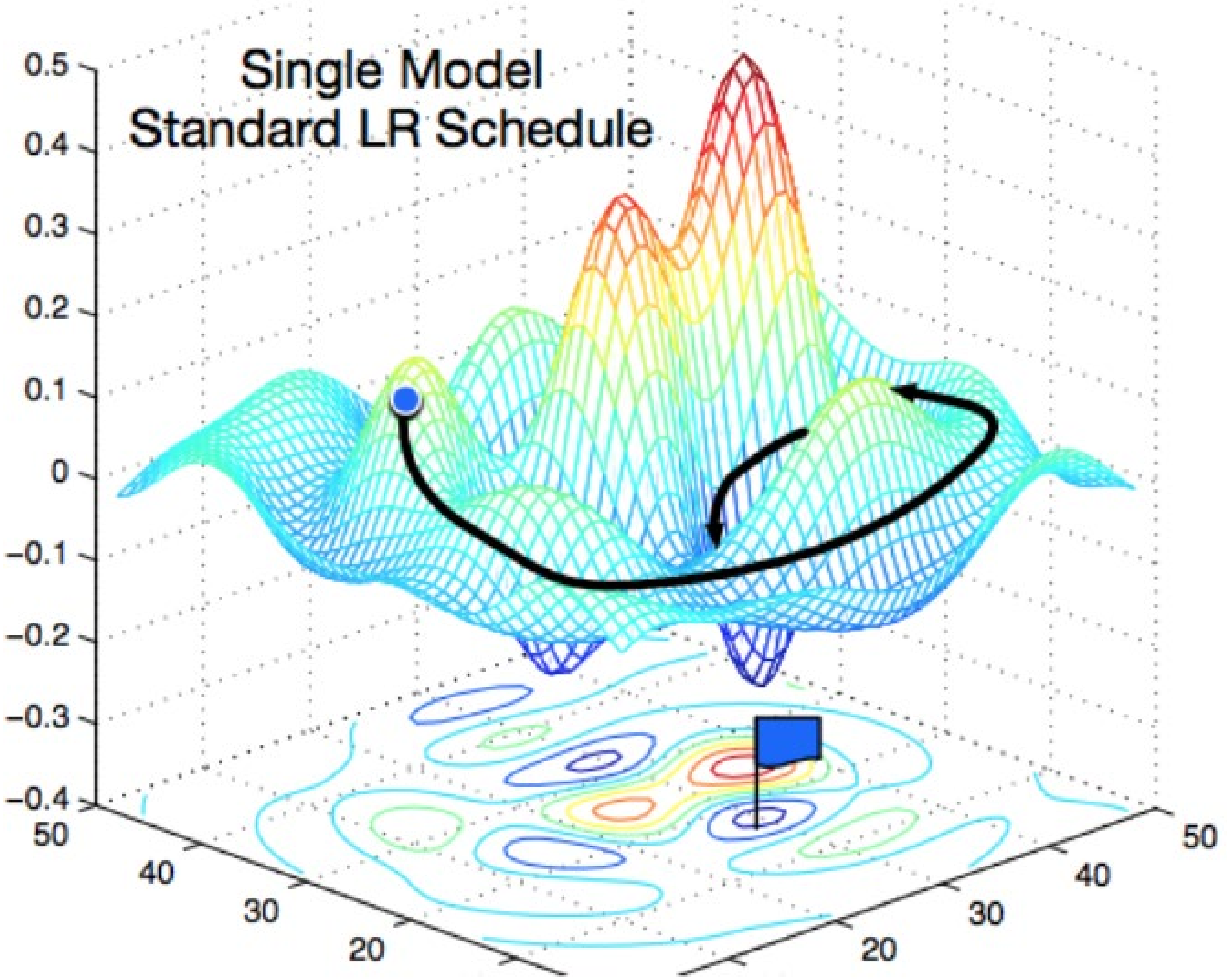
gradient on the top x gradient from the current operation

$$\frac{\partial L}{\partial \boldsymbol{W}} = \frac{\partial L}{\partial \boldsymbol{z_1}} \frac{\partial \boldsymbol{z_1}}{\partial \boldsymbol{W}}$$



$$\mathbf{a} = sigmoid(\mathbf{Wx} + \mathbf{b})$$

Non-convex Optimization



[Gao and Li et al., 2018]

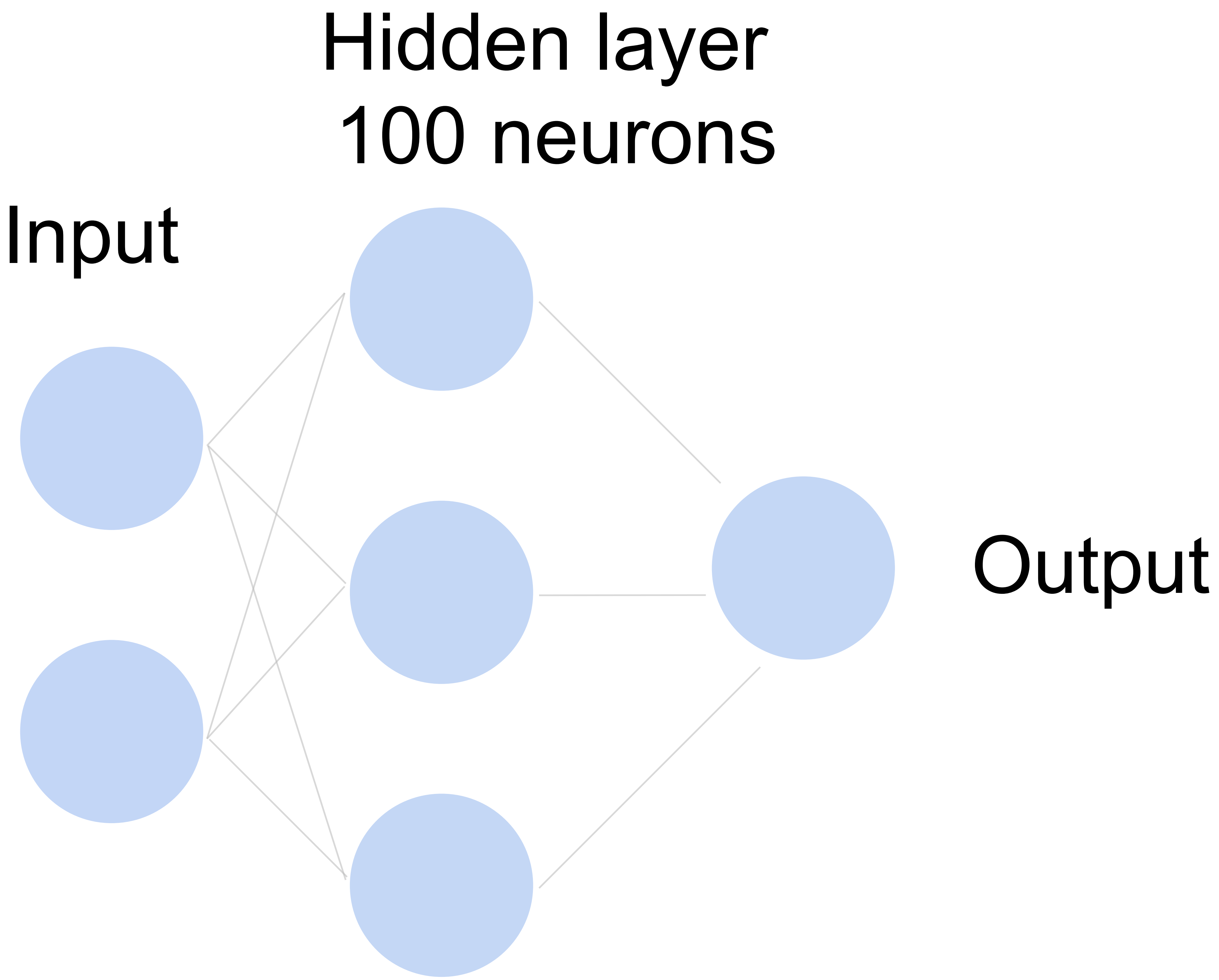
How to classify

Cats vs. dogs?

36M floats in a RGB image!

Fully Connected Networks

Cats vs. dogs?



~ 36M elements x 100 = **~3.6B** parameters!

Convolutions come to rescue!

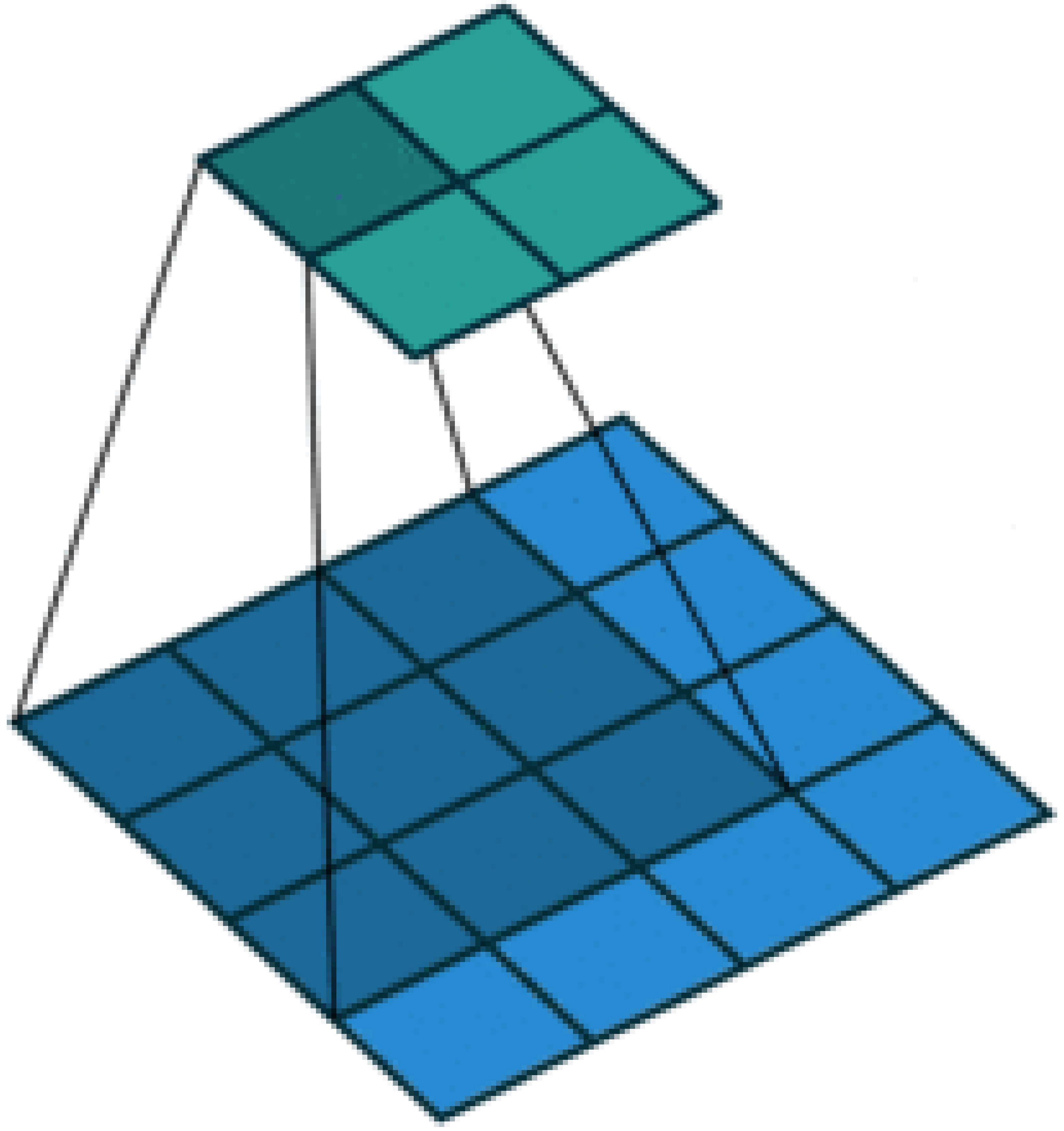
Where is Waldo?

Why Convolution?

- Translation Invariance
- Locality

2-D Convolution

$$\underset{\text{Input}}{\begin{bmatrix} 0 & 1 & 2 \\ 3 & 4 & 5 \\ 6 & 7 & 8 \end{bmatrix}} * \underset{\text{Kernel}}{\begin{bmatrix} 0 & 1 \\ 2 & 3 \end{bmatrix}} = \underset{\text{Output}}{\begin{bmatrix} 19 & 25 \\ 37 & 43 \end{bmatrix}}$$



(vdumoulin@ Github)

$$0 \times 0 + 1 \times 1 + 3 \times 2 + 4 \times 3 = 19,$$
$$1 \times 0 + 2 \times 1 + 4 \times 2 + 5 \times 3 = 25,$$
$$3 \times 0 + 4 \times 1 + 6 \times 2 + 7 \times 3 = 37,$$
$$4 \times 0 + 5 \times 1 + 7 \times 2 + 8 \times 3 = 43.$$

2-D Convolution Layer

$$\begin{bmatrix}0 & 1 & 2\\ 3 & 4 & 5\\ 6 & 7 & 8\end{bmatrix} * \begin{bmatrix}0 & 1\\ 2 & 3\end{bmatrix} = \begin{bmatrix}19 & 25\\ 37 & 43\end{bmatrix}$$

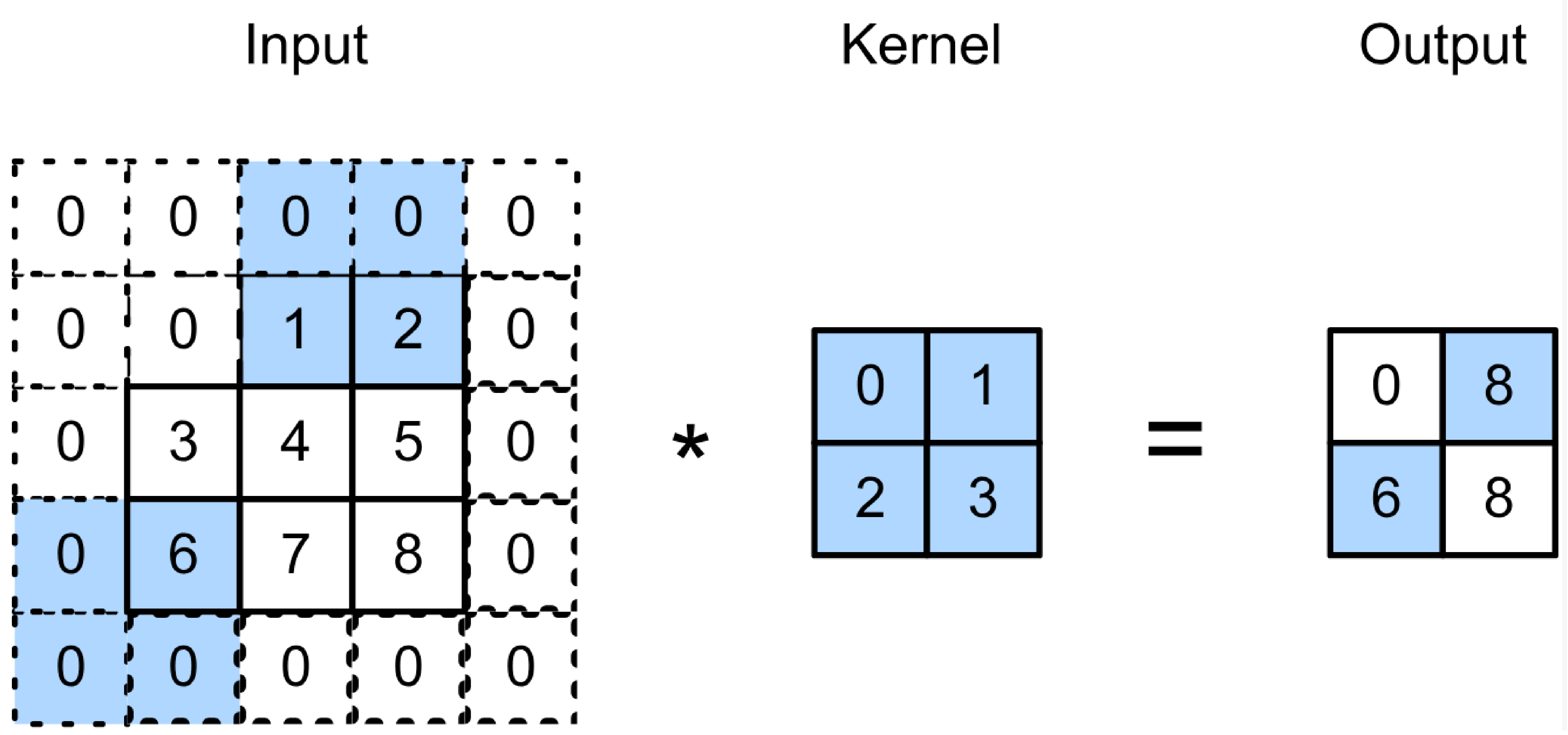
- $\mathbf{X}$: $n_h \times n_w$ input matrix
- $\mathbf{W}$: $k_h \times k_w$ kernel matrix
- b: scalar bias
- $\mathbf{Y}$: $(n_h - k_h + 1) \times (n_w - k_w + 1)$ output matrix

$$\mathbf{Y} = \mathbf{X} \star \mathbf{W} + b$$

- **W** and *b* are learnable parameters

2-D Convolution Layer with Stride and Padding

- Stride is the #rows/#columns per slide
- Padding adds rows/columns around input
- Output shape



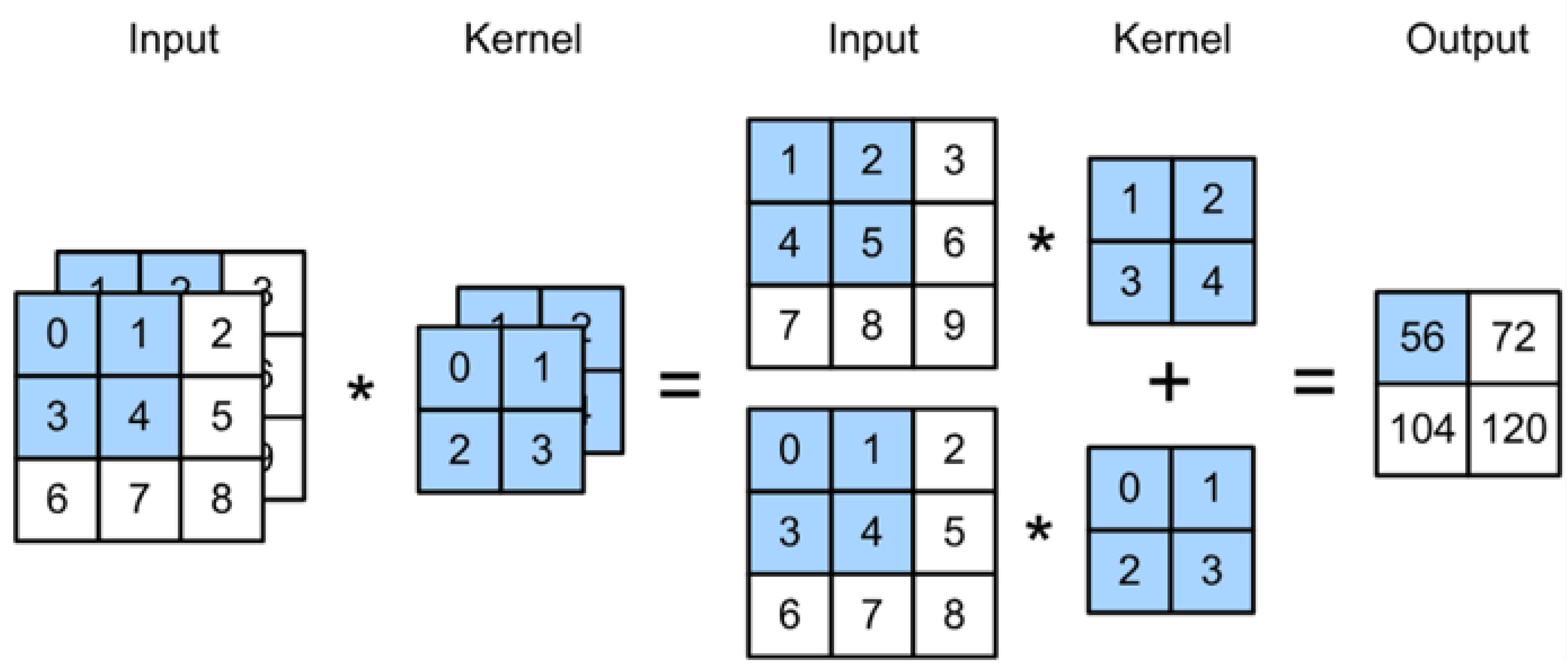
Kernel/filter size

$$\lfloor (n_h - k_h + p_h + s_h)/s_h \rfloor \times \lfloor (n_w - k_w + p_w + s_w)/s_w \rfloor$$

Input size **Pad** **Stride**

Multiple Input Channels

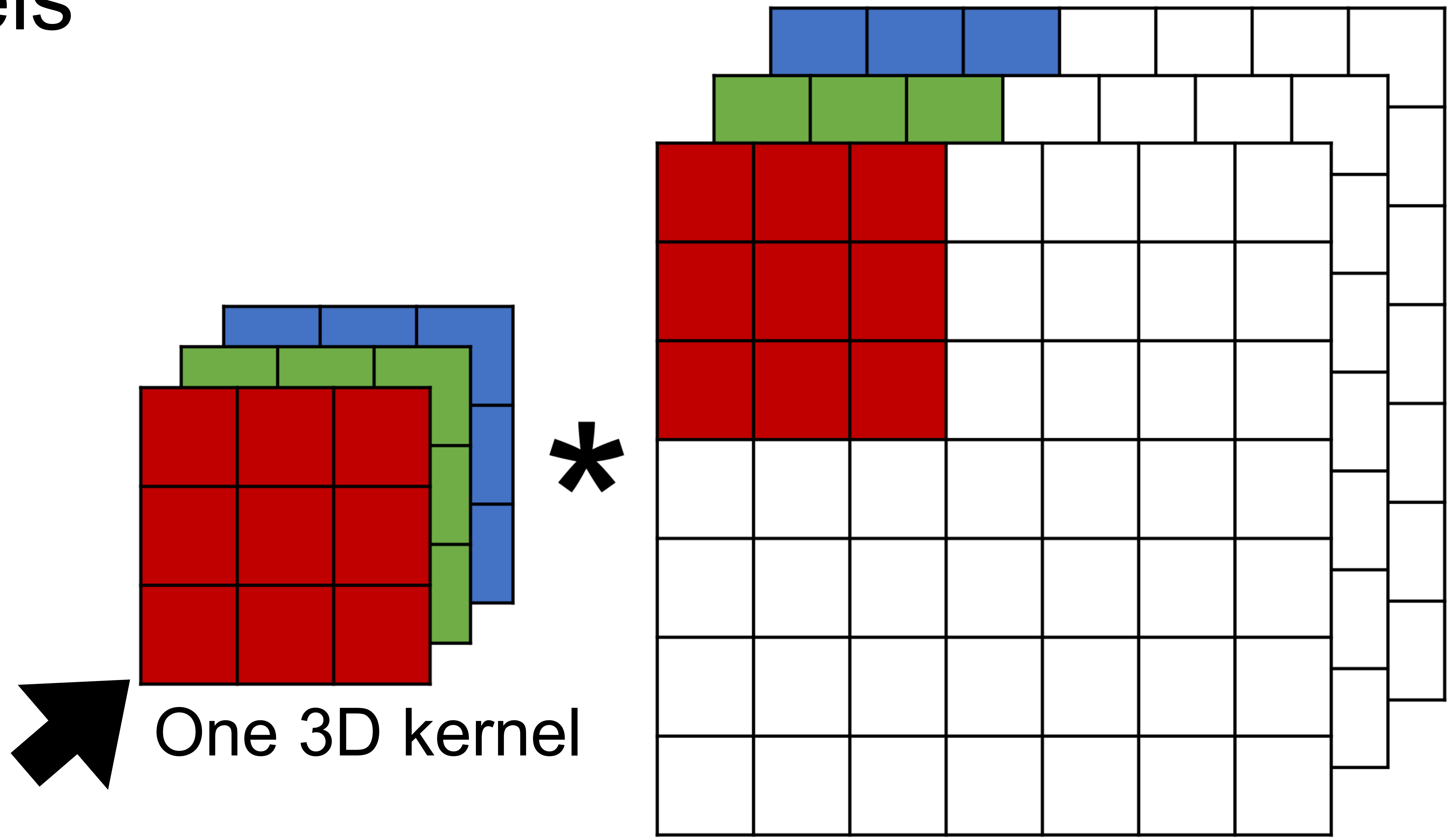
- Input and kernel can be 3D, e.g., an RGB image have 3 channels
- Have a kernel for each channel, and then sum results over channels



$$(1 \times 1 + 2 \times 2 + 4 \times 3 + 5 \times 4)$$
$$+(0 \times 0 + 1 \times 1 + 3 \times 2 + 4 \times 3)$$
$$= 56$$

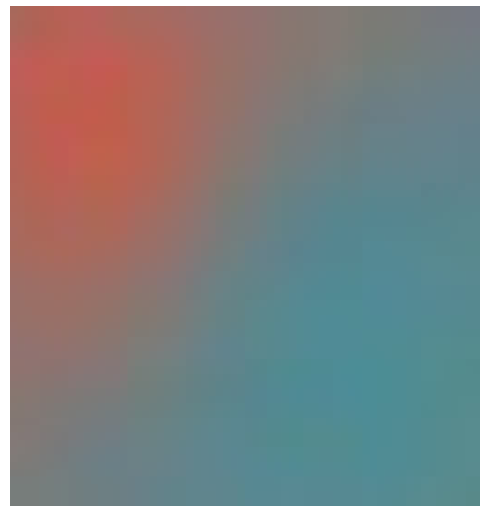
Multiple Input Channels

- Input and kernel can be 3D, e.g., an RGB image have 3 channels
- Have a 2D kernel for each channel, and then sum results over channels



Multiple Input Channels

- Input and kernel can be 3D, e.g., an RGB image have 3 channels
- Also call each 3D kernel a "**filter**", which produce only **one** output channel (due to summation over channels)



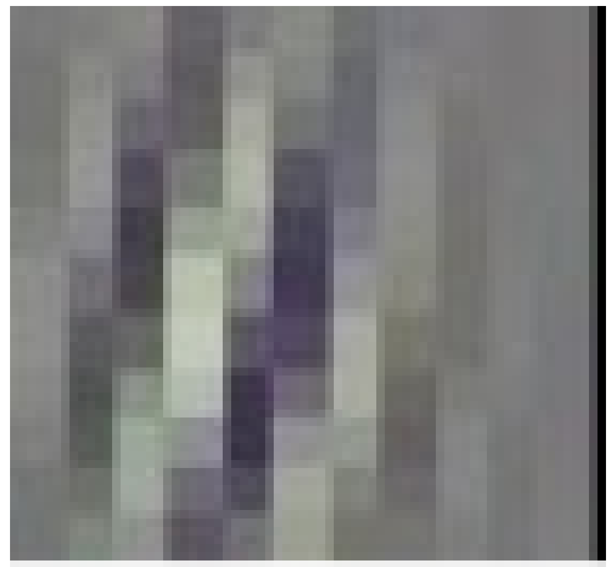
*

One filter
(3 channels)

RGB (3 input channels)

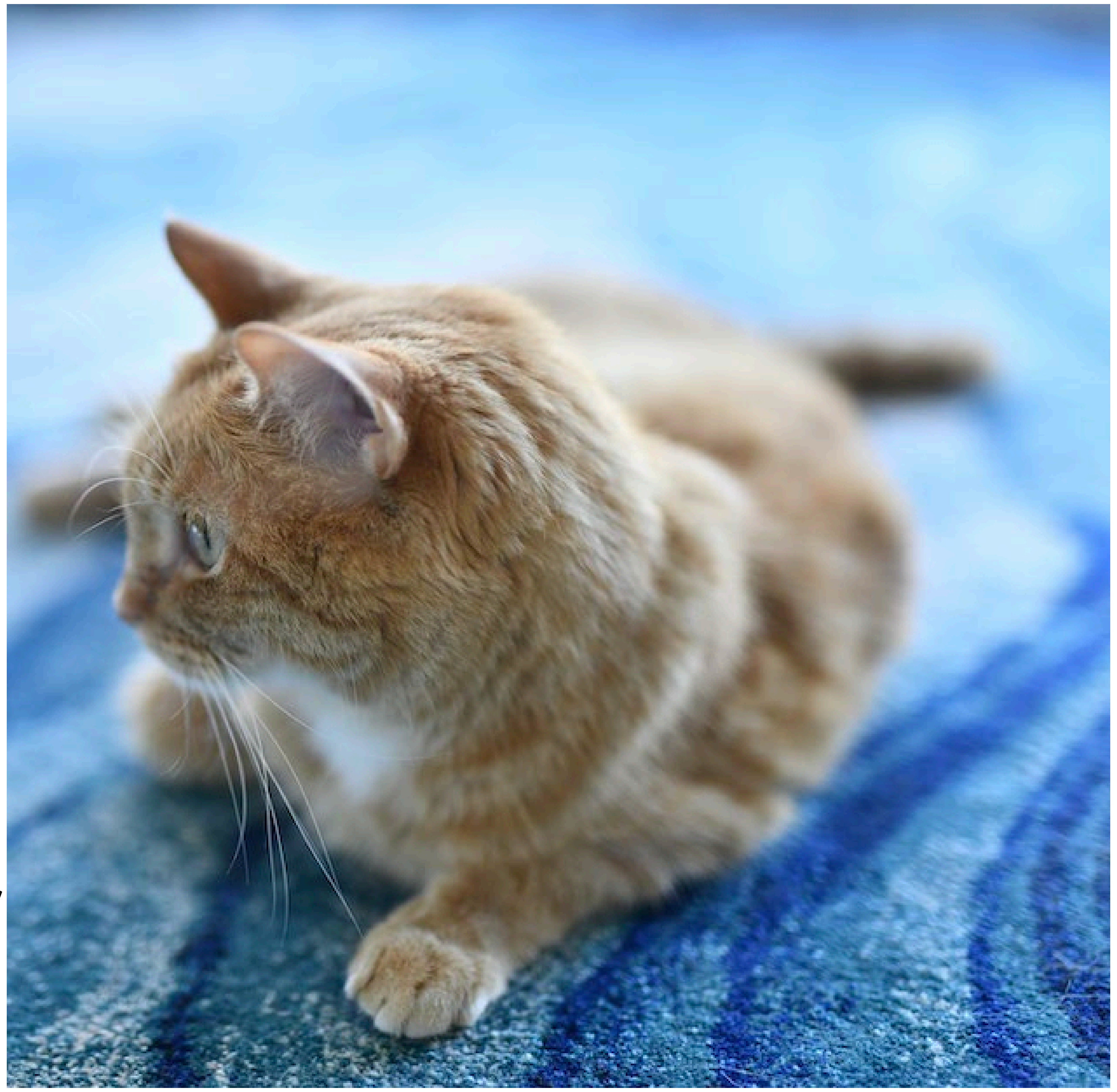
Multiple filters (in one layer)

- Apply multiple filters on the input
- Each filter may learn different features about the input
- Each filter (3D kernel) produces one output channel



A different filter

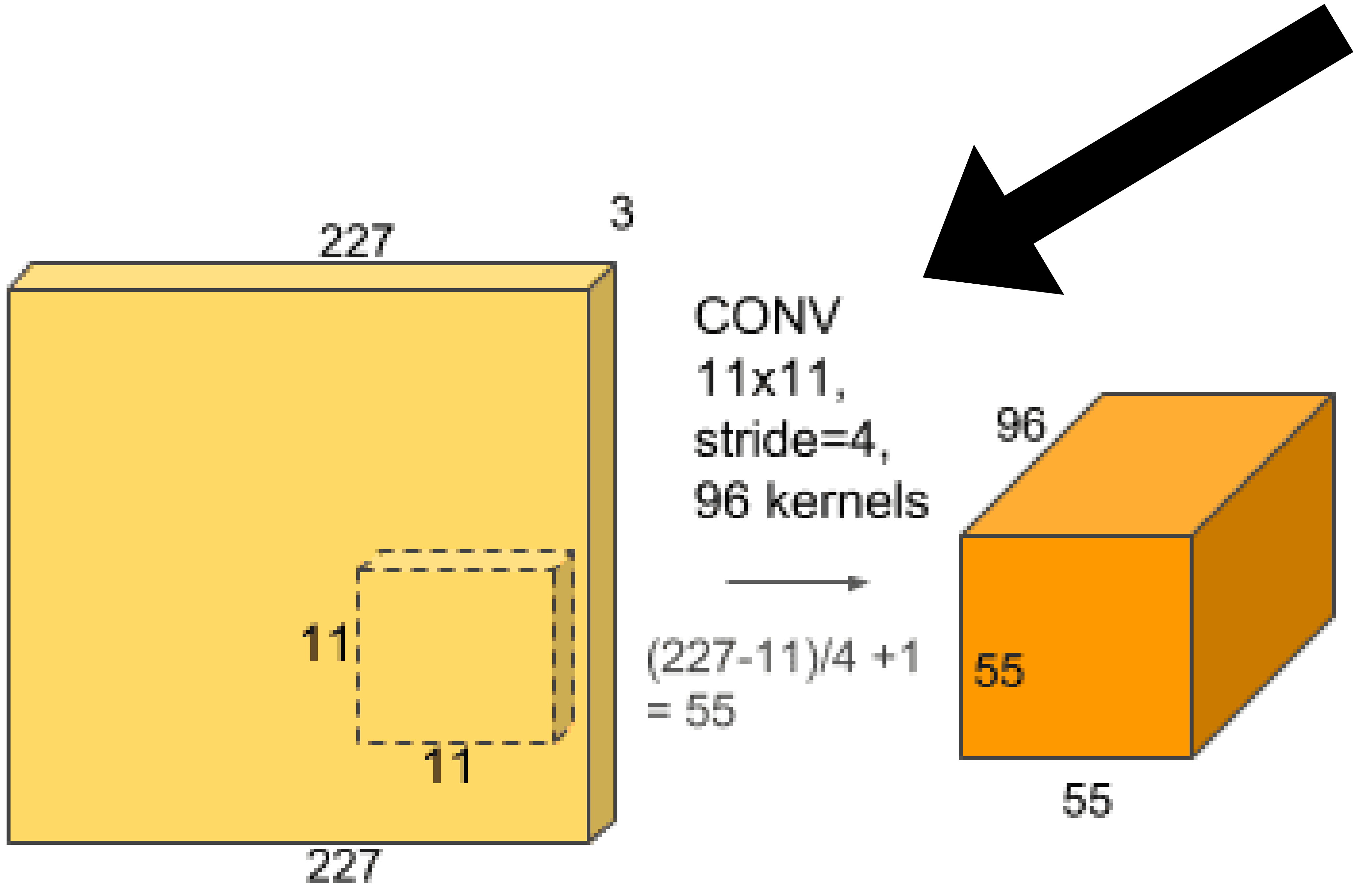
*

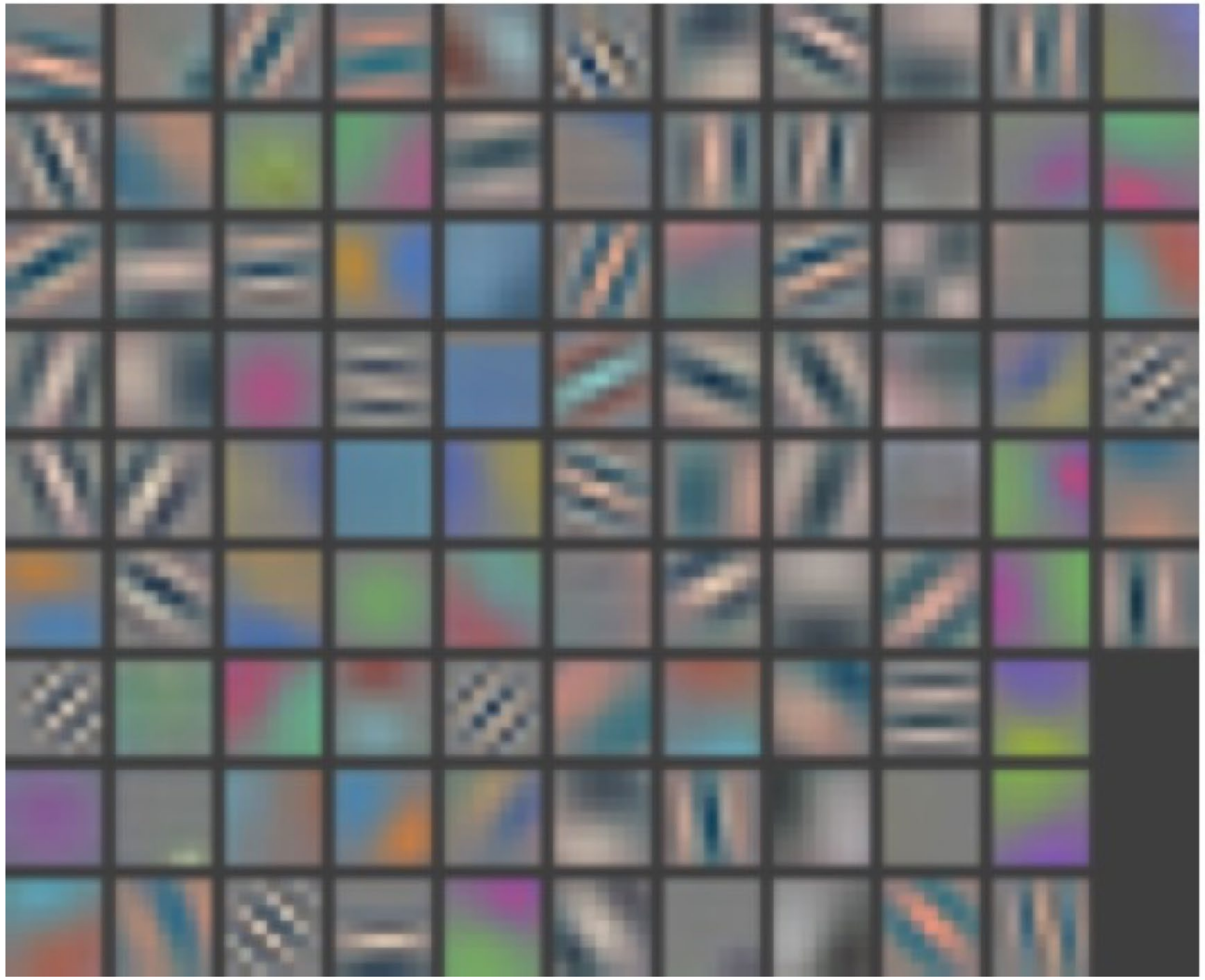


RGB (3 input channels)

Conv1 Filters in AlexNet

- 96 filters (each of size 11x11x3)
- Gabor filters





Figures from Visualizing and Understanding Convolutional Networks
by *M. Zeiler and R. Fergus*

Multiple Output Channels

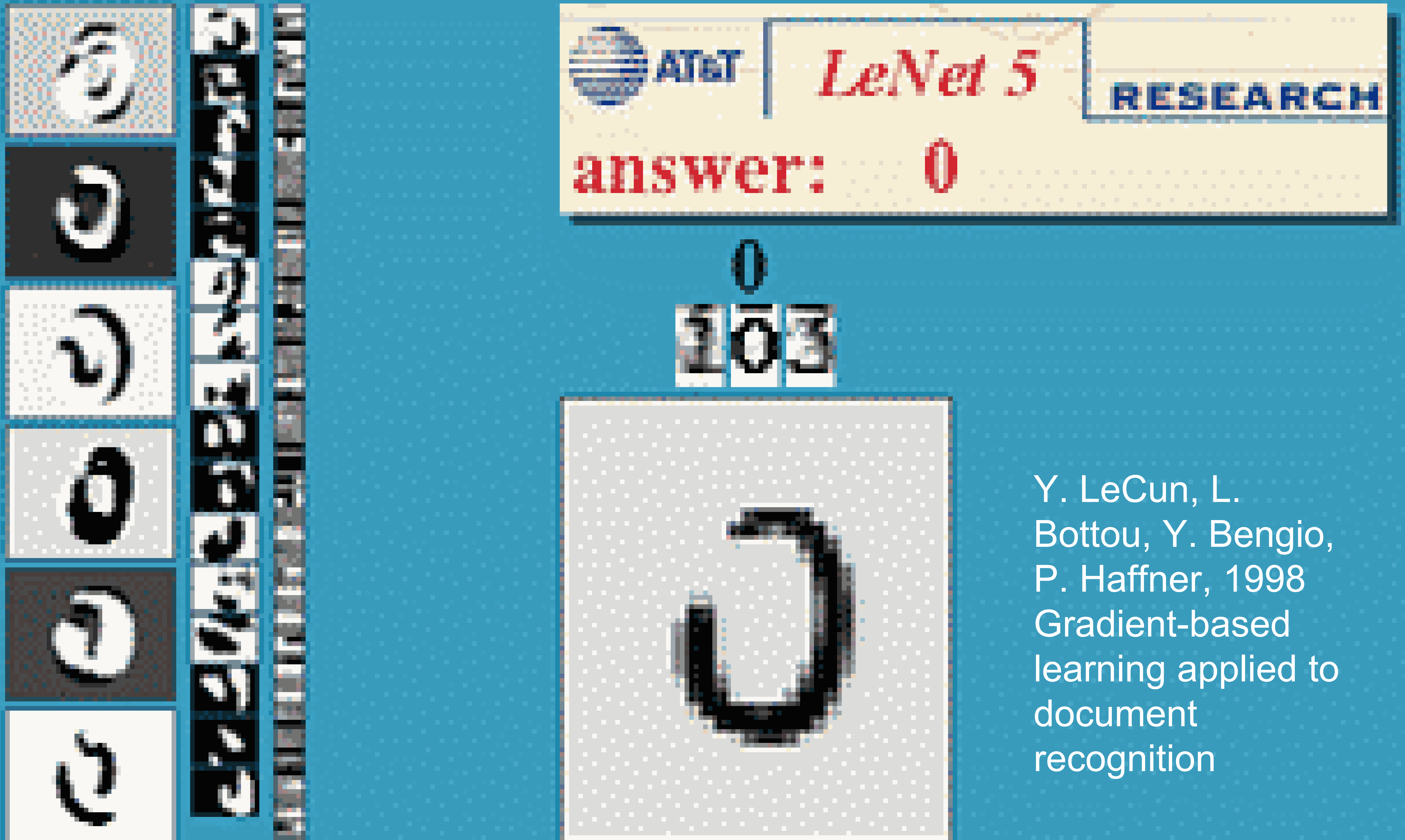
- The # of output channels = # of filters
- Input $\mathbf{X}$: $c_i \times n_h \times n_w$
- Kernel $\mathbf{W}$: $c_o \times c_i \times k_h \times k_w$
- Output $\mathbf{Y}$: $c_o \times m_h \times m_w$

$$\mathbf{Y}_{i,:,:} = \mathbf{X} \star \mathbf{W}_{i,:,:,:}$$
$$for\, i = 1, \ldots, c_o$$

Convolutional Neural Networks

LeNet Architecture

gluon-cv.mxnet.io



Y. LeCun, L. Bottou, Y. Bengio, P. Haffner, 1998 Gradient-based learning applied to document recognition

Quiz break

Which one of the following is NOT true?

A. LeNet has two convolutional layers

B. The first convolutional layer in LeNet has 5x5x6x3 parameters, in case of RGB input

C. Pooling is performed right after convolution

D. Pooling layer does not have learnable parameters

Quiz break

Which one of the following is NOT true?

A. LeNet has two convolutional layers

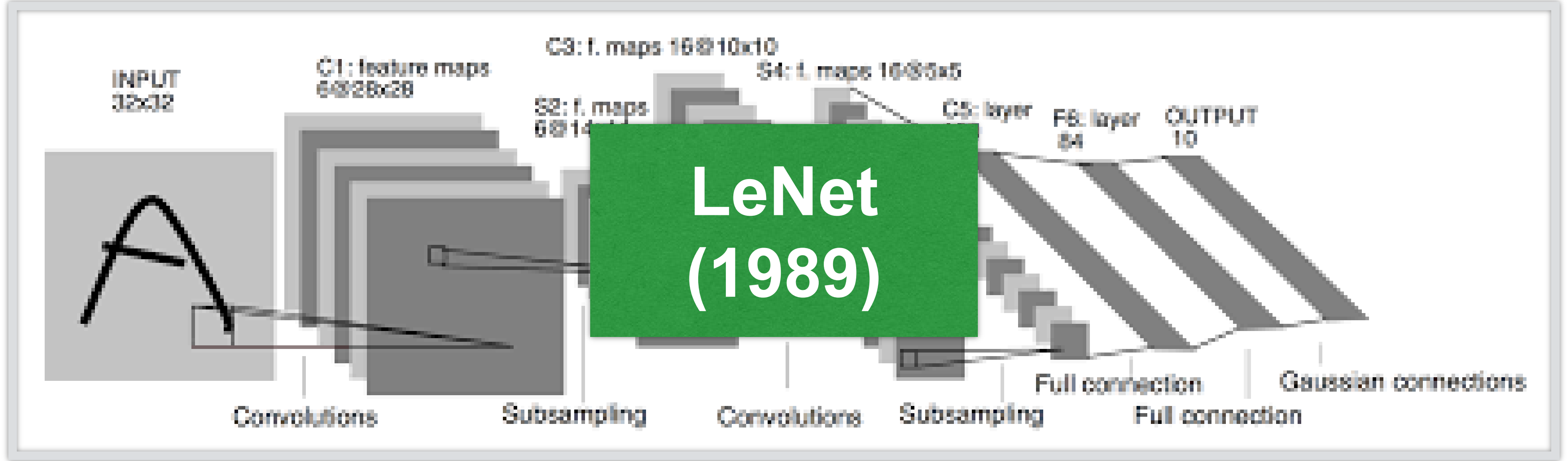
B. The first convolutional layer in LeNet has 5x5x6x3 parameters, in case of RGB input

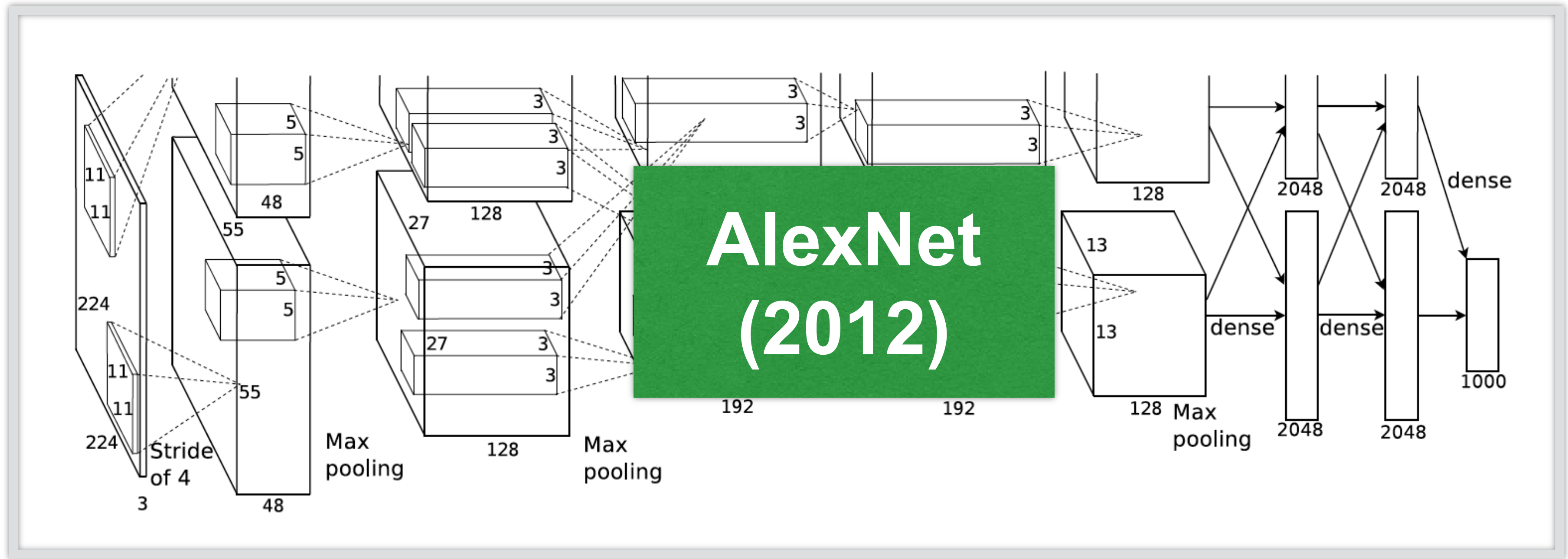
C. Pooling is performed right after convolution

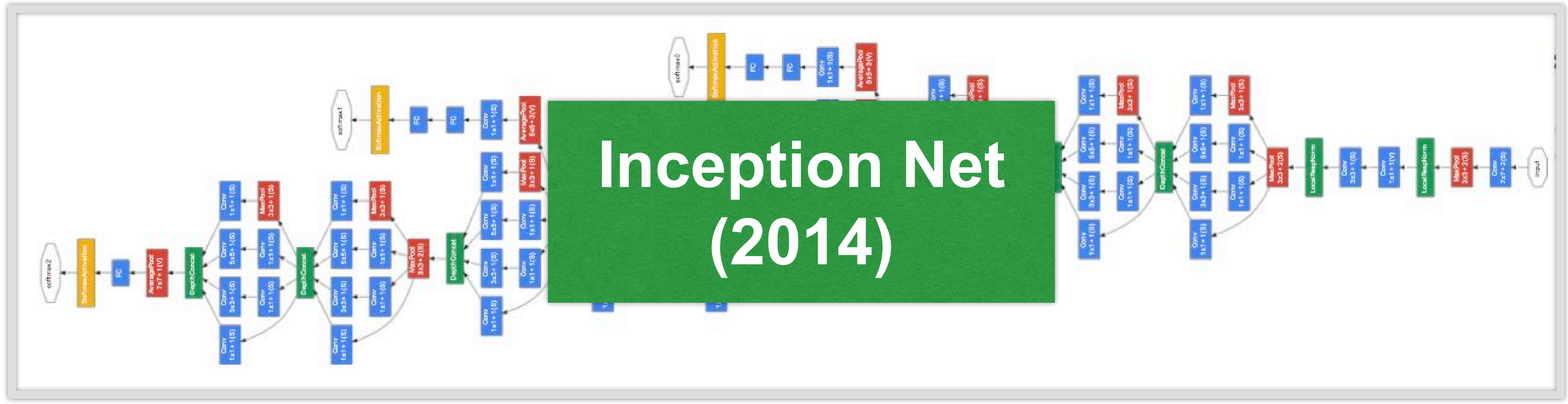
D. Pooling layer does not have learnable parameters

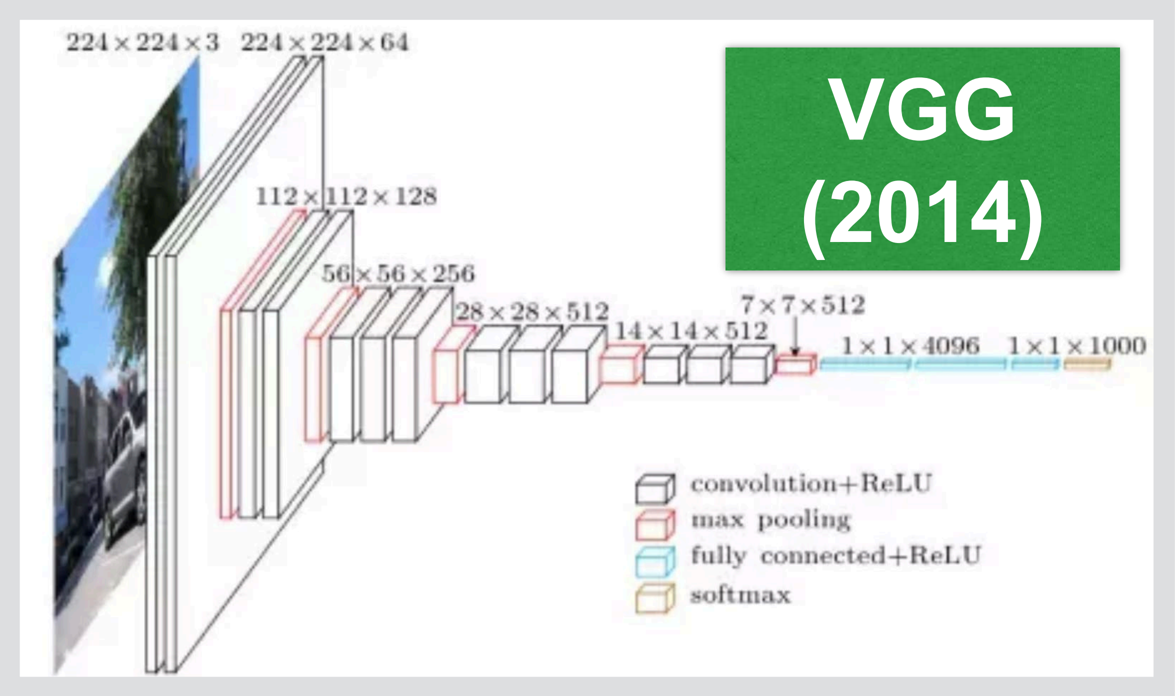
Pooling is performed after ReLU: conv -> relu -> pooling

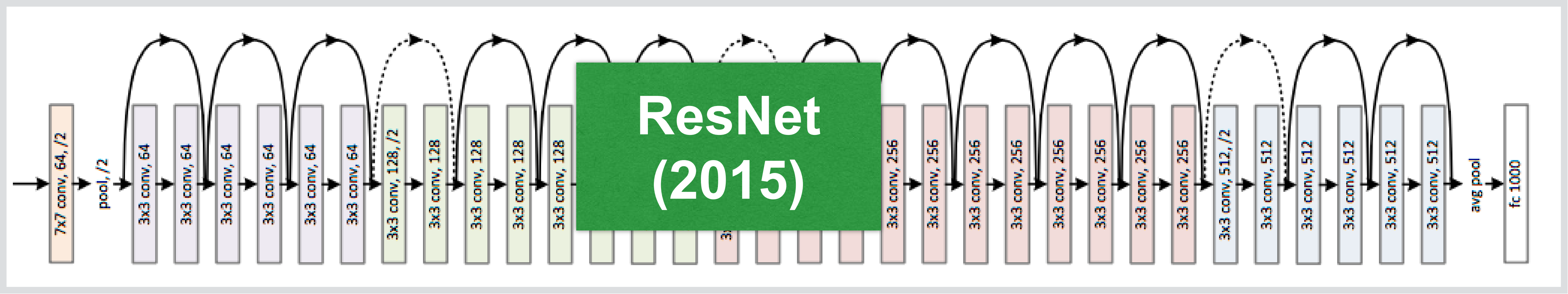
Evolution of neural net architectures

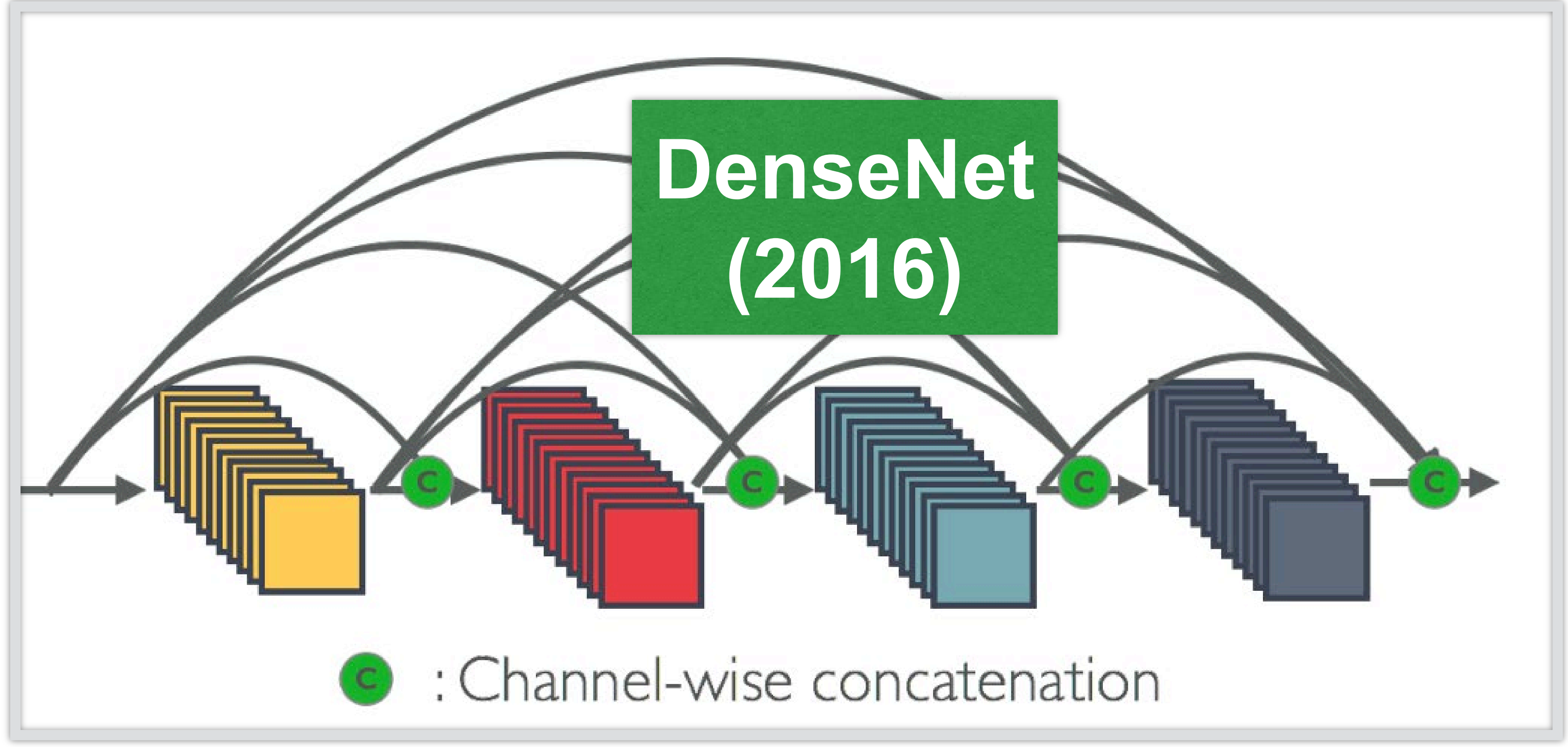






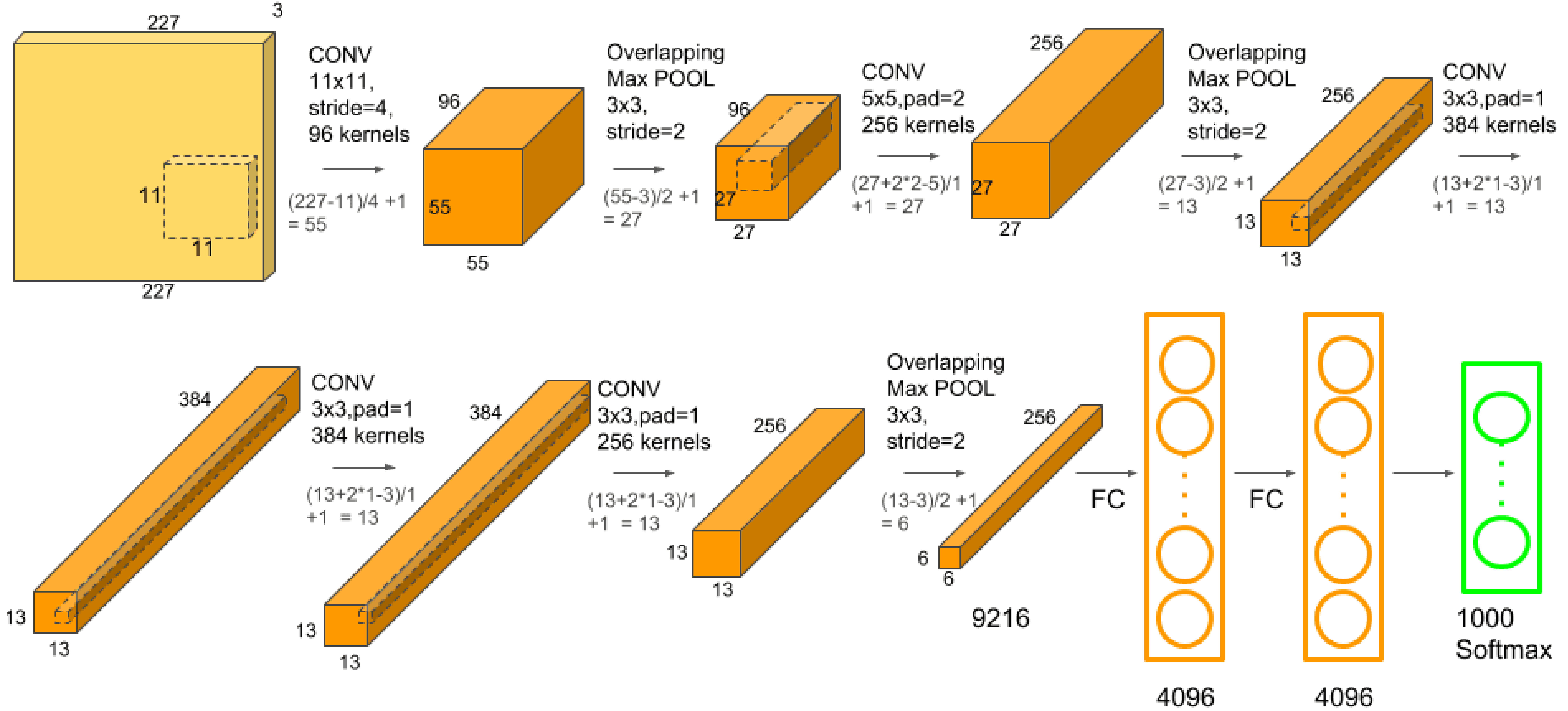






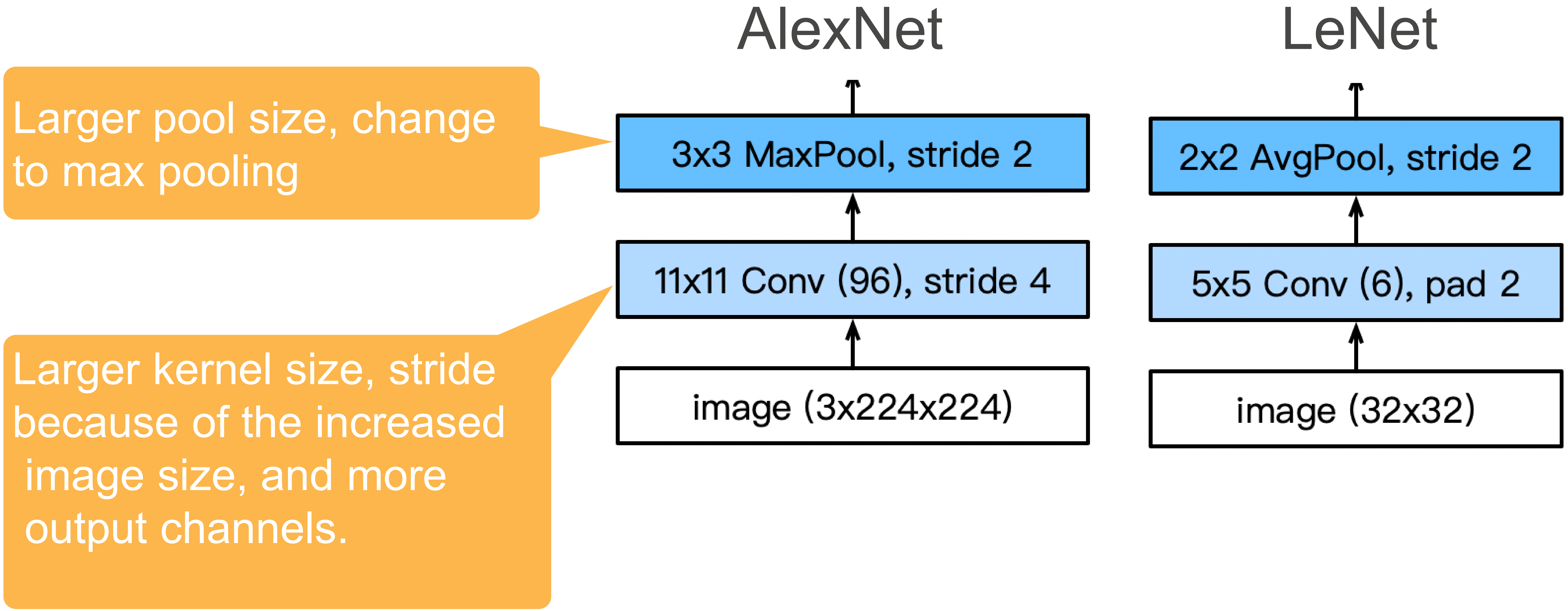
Deng et al. 2009

AlexNet

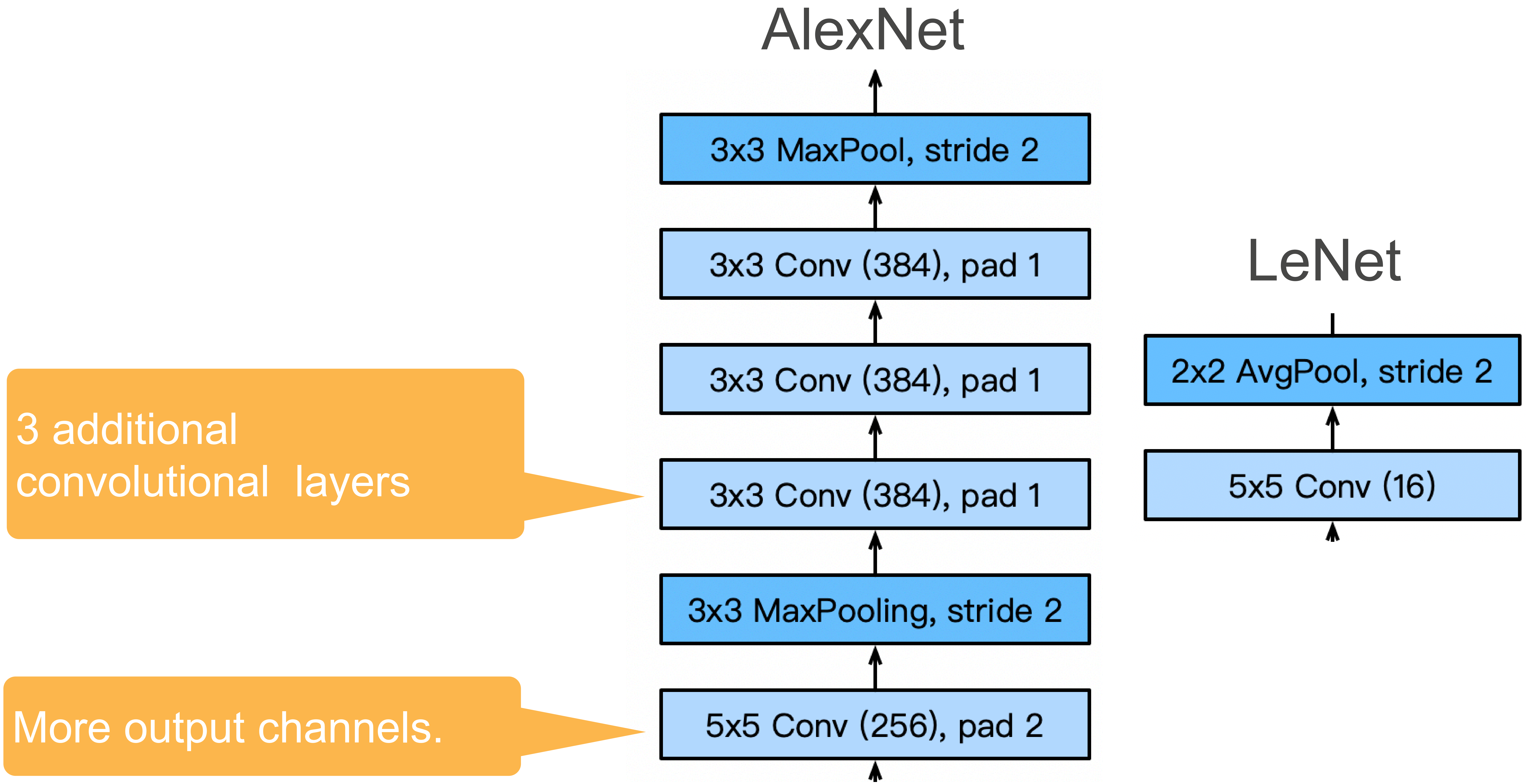


[Krizhevsky et al. 2012]

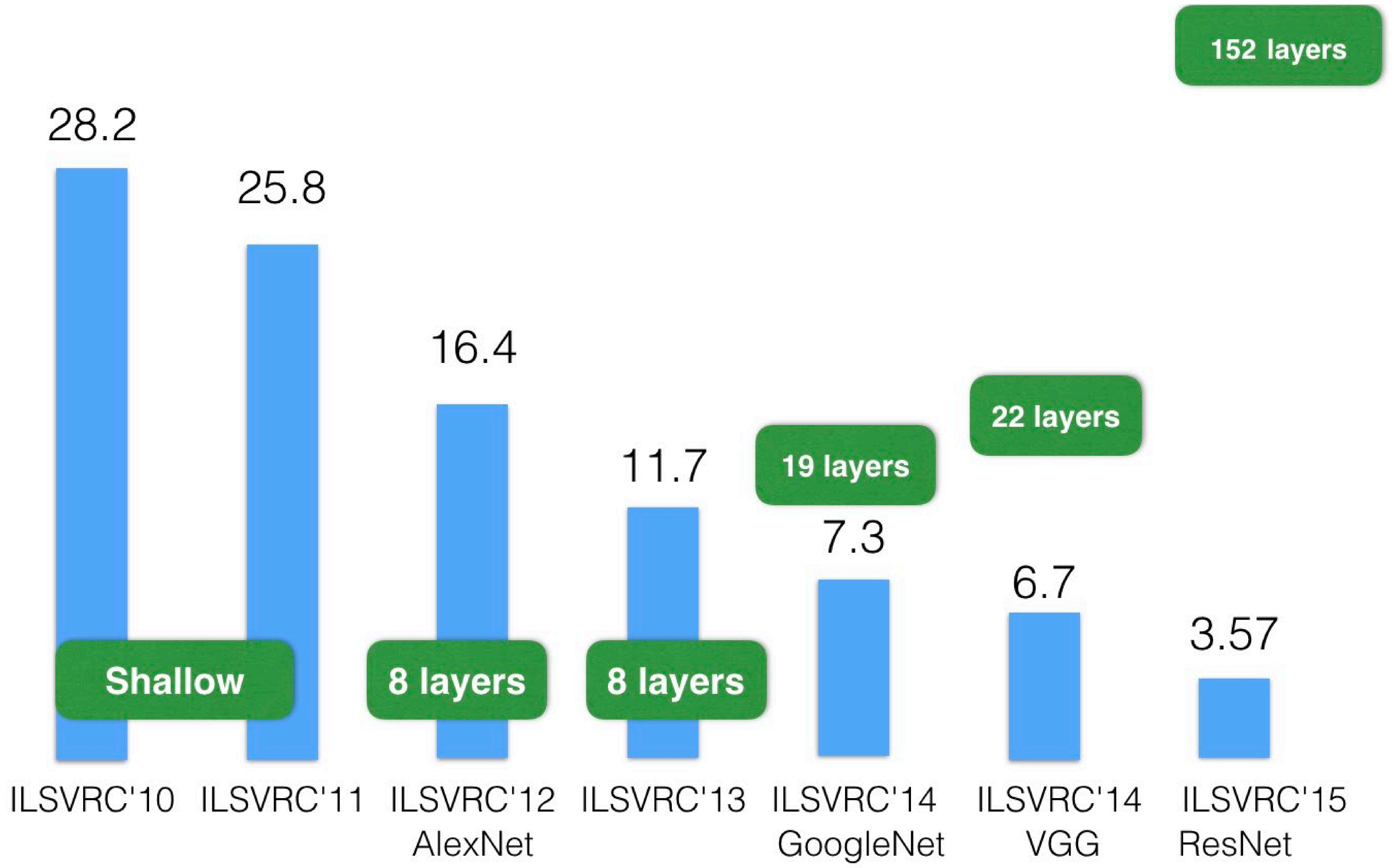
AlexNet vs LeNet Architecture



AlexNet Architecture



ResNet: Going deeper in depth



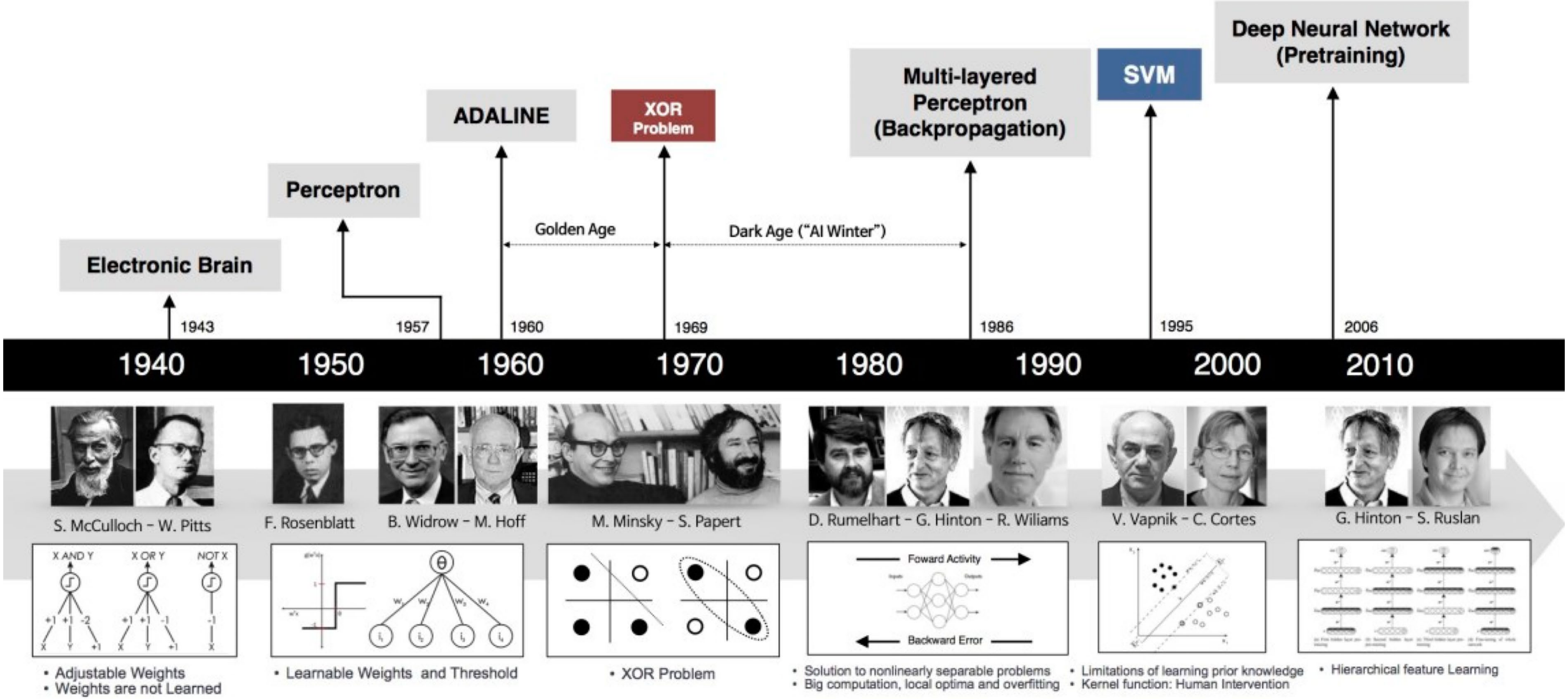
ImageNet Top-5 error%

[He et al. 2015]

Other neural network architectures

- Convolutional neural networks are one of many special types of layers.
  - Main use is for processing images.
  - Also can be useful for handling time series.
- Other common architectures:
  - Recurrent neural networks: hidden activations are a function of input and activations from previous inputs. Designed for sequential data such as text.
  - Graph neural networks: take graph data as input.
  - Transformers: take sequences as input and learn what parts of input to pay attention to.

Brief history of neural networks



What we’ve learned today…

- Modeling a single neuron
  - Linear perceptron
  - Limited power of a single neuron
- Multi-layer perceptron
- Training of neural networks
  - Loss function (cross entropy)
  - Backpropagation and SGD
- Convolutional neural networks
  - Convolution, pooling, stride, padding
  - Basic architectures (LeNet etc.)
  - More advanced architectures (AlexNet, ResNet etc)

Thank you!

Some of the slides in these lectures have been adapted from materials developed by Alex Smola and Mu Li:

https://courses.d2l.ai/berkeley-stat-157/index.html