



CS540 Introduction to Artificial Intelligence (Deep) Neural Networks Summary

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Nov 9, 2021

How to classify

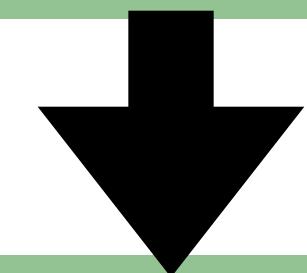
Cats vs. dogs?



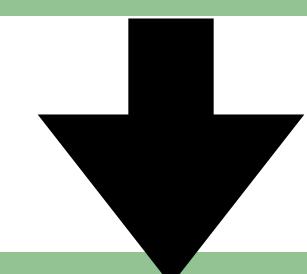
How to classify Cats vs. dogs?



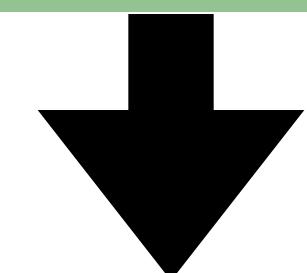
Single-layer
Perceptron



Multi-layer
Perceptron



Training of neural
networks



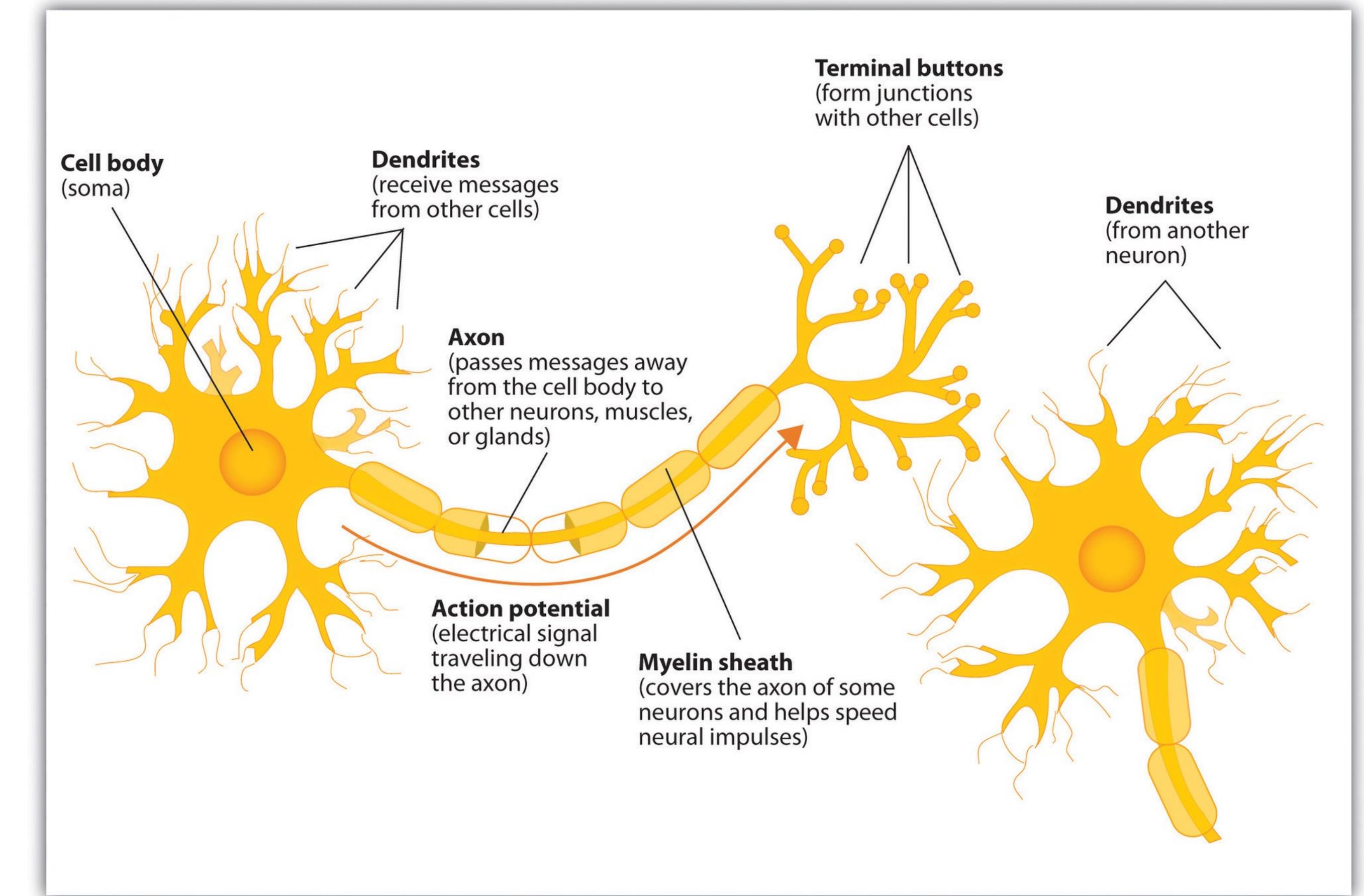
Convolutional
neural networks

Inspiration from neuroscience

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



(wikipedia)



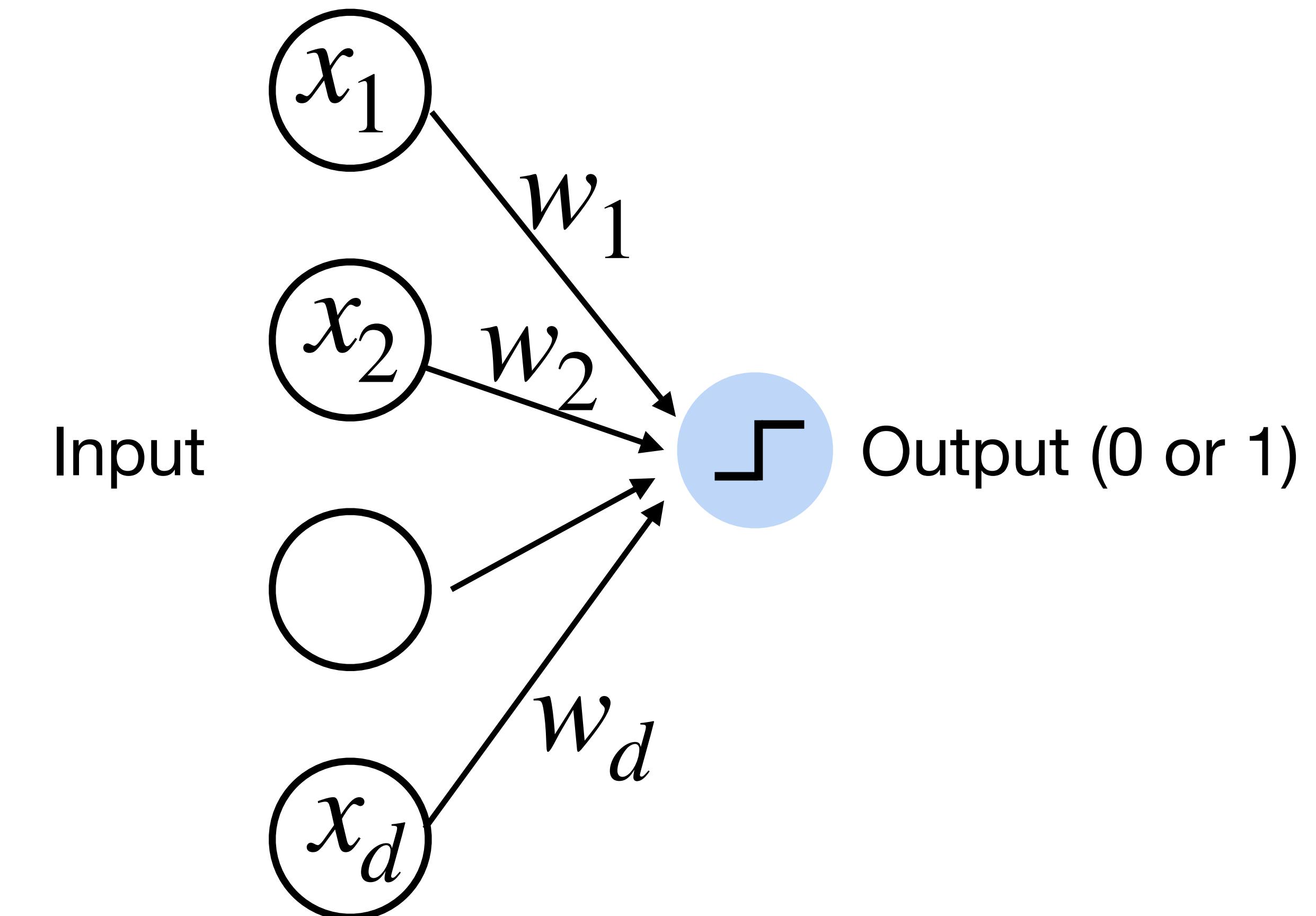
Perceptron

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

$$o = \sigma(\mathbf{w}^\top \mathbf{x} + b)$$

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

Cats vs. dogs?



Perceptron

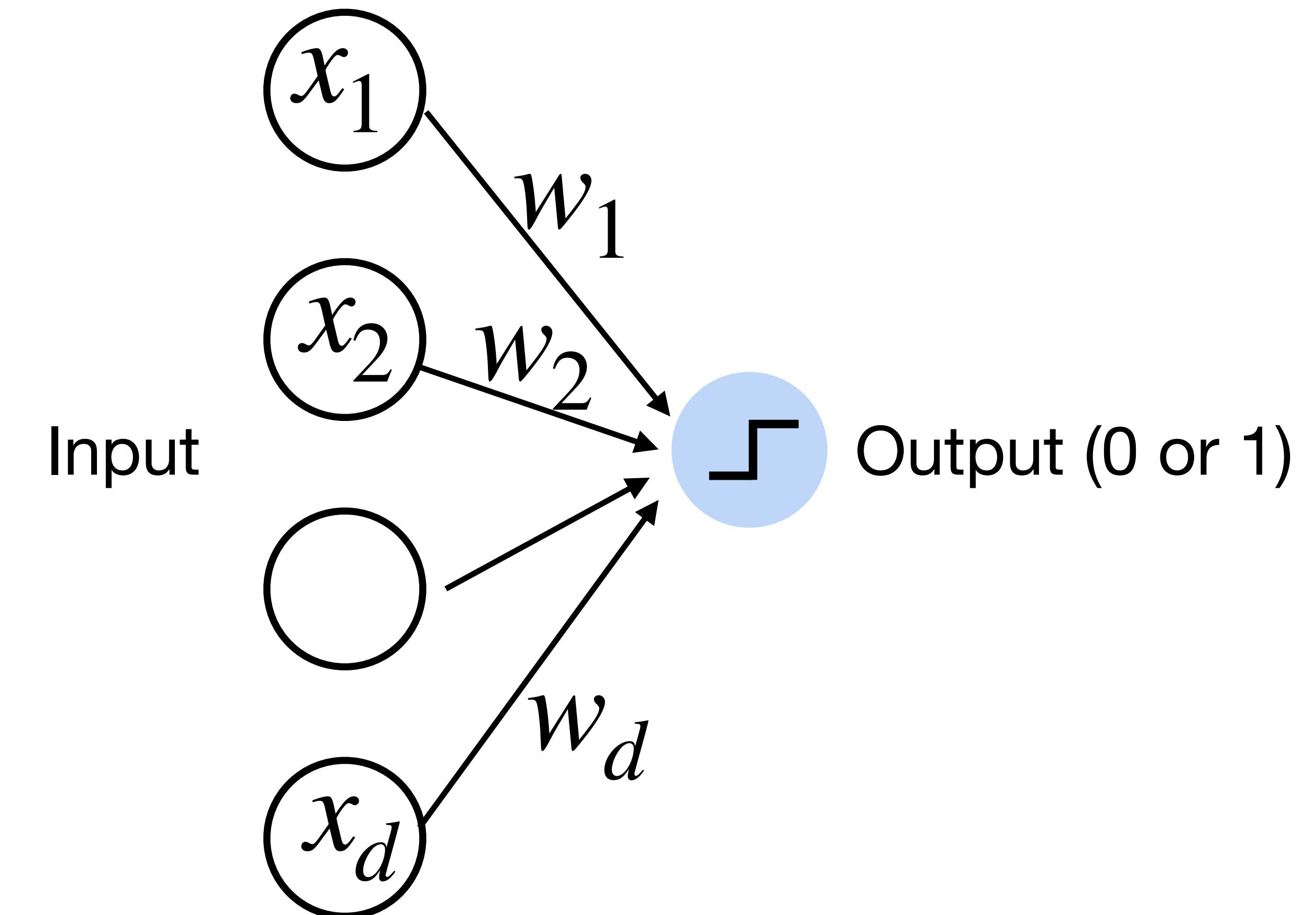
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Activation function

Cats vs. dogs?



Training the Perceptron

Perceptron Algorithm

```
Initialize  $\vec{w} = \vec{0}$                                 // Initialize  $\vec{w}$ .  $\vec{w} = \vec{0}$  misclassifies everything.  
while TRUE do                                // Keep looping  
     $m = 0$                                          // Count the number of misclassifications,  $m$   
    for  $(x_i, y_i) \in D$  do                      // Loop over each (data, label) pair in the dataset,  $D$   
        if  $o_i \neq y_i$  then                         // If the pair  $(\vec{x}_i, y_i)$  is misclassified  
             $\vec{w} \leftarrow \vec{w} + x_i$  if  $y_i = 1$ ,  $\vec{w} \leftarrow \vec{w} - x_i$  if  $y_i = 0$   
             $m \leftarrow m + 1$                           // Counter the number of misclassification  
        end if  
    end for  
    if  $m = 0$  then                            // If the most recent  $\vec{w}$  gave 0 misclassifications  
        break                                     // Break out of the while-loop  
    end if  
end while                                    // Otherwise, keep looping!
```

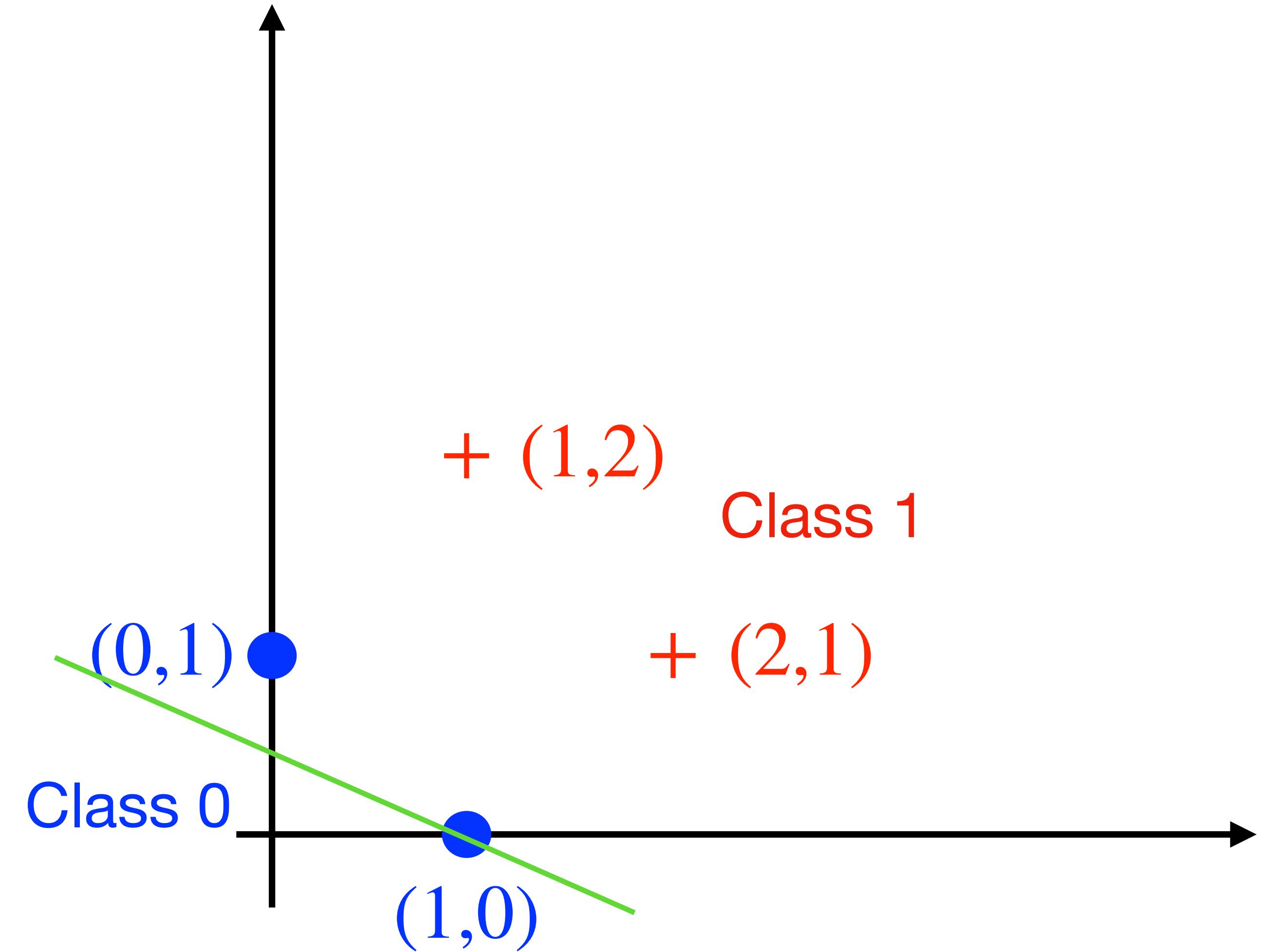
For simplicity, the weight vector and input vector are extended vectors (including the bias or the constant 1).

Example: Training the Perceptron

- Suppose we begin with:

$$\mathbf{w} = (1,2), b = -1$$

- Extended vectors:



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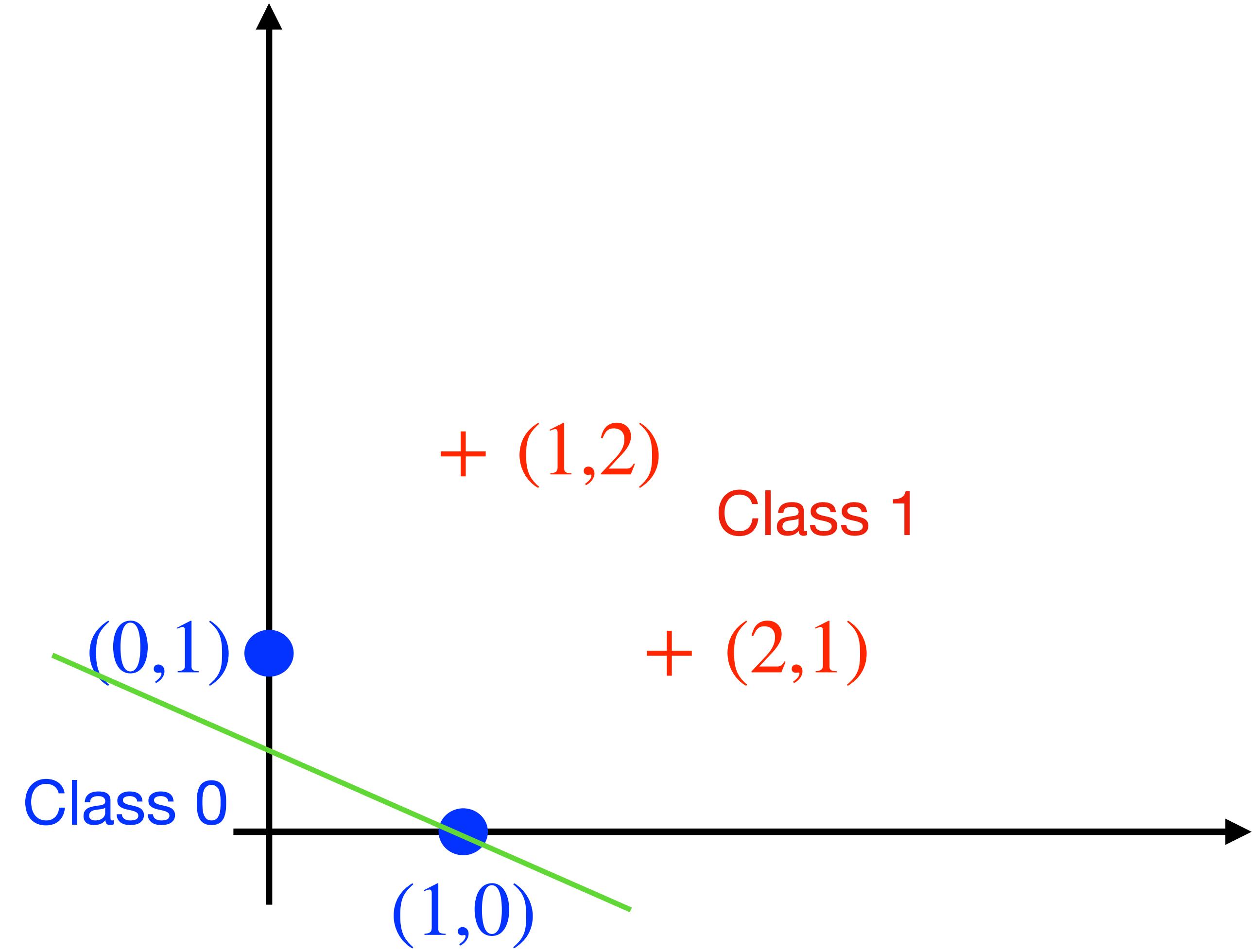
$$\vec{w} = (1, 2, -1)$$

$$\vec{x}_1 = (0, 1, 1)$$

$$\vec{x}_2 = (1, 0, 1)$$

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$$\vec{x}_4 = (1, 2, 1)$$

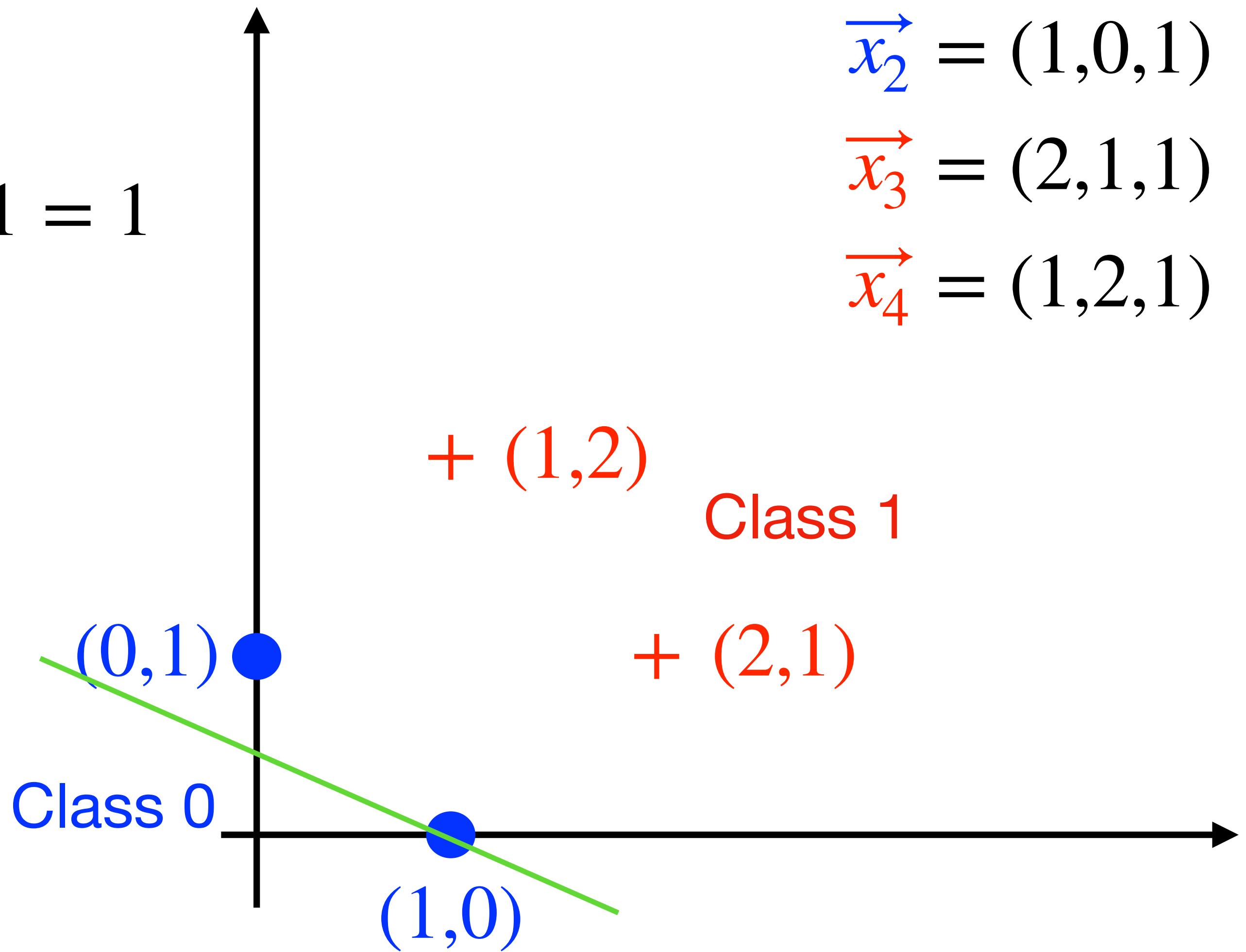


Example: Training the Perceptron

- First Epoch:

$$\vec{x}_1 : \langle \vec{w}, \vec{x}_1 \rangle = 1 \times 0 + 2 \times 1 + (-1) \times 1 = 1$$

$$\begin{aligned}\vec{w} &= (1, 2, -1) \\ \vec{x}_1 &= (0, 1, 1) \\ \vec{x}_2 &= (1, 0, 1) \\ \vec{x}_3 &= (2, 1, 1) \\ \vec{x}_4 &= (1, 2, 1)\end{aligned}$$



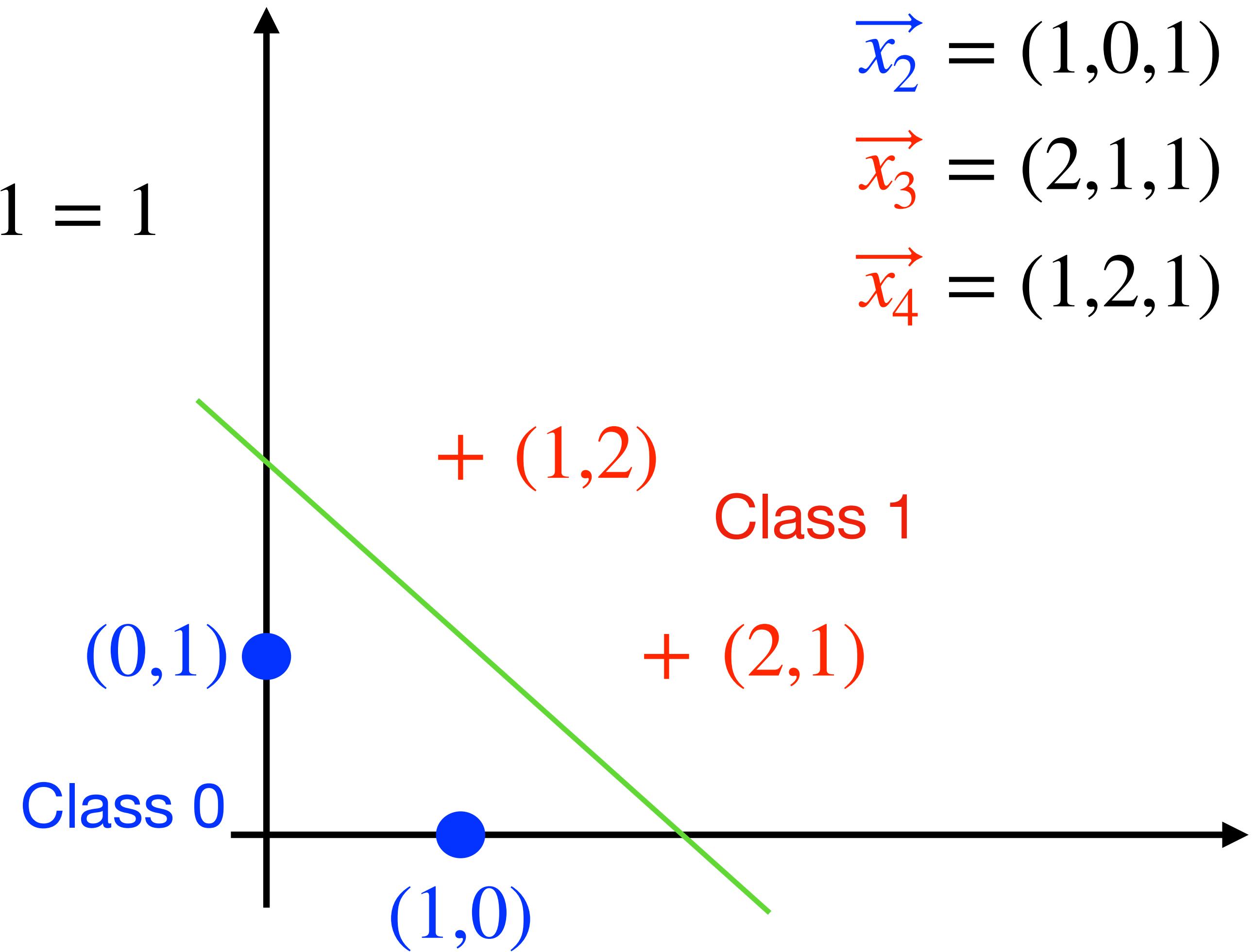
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wrong prediction

update $\vec{w} \leftarrow \vec{w} - \vec{x}_1 = (1, 1, -2)$



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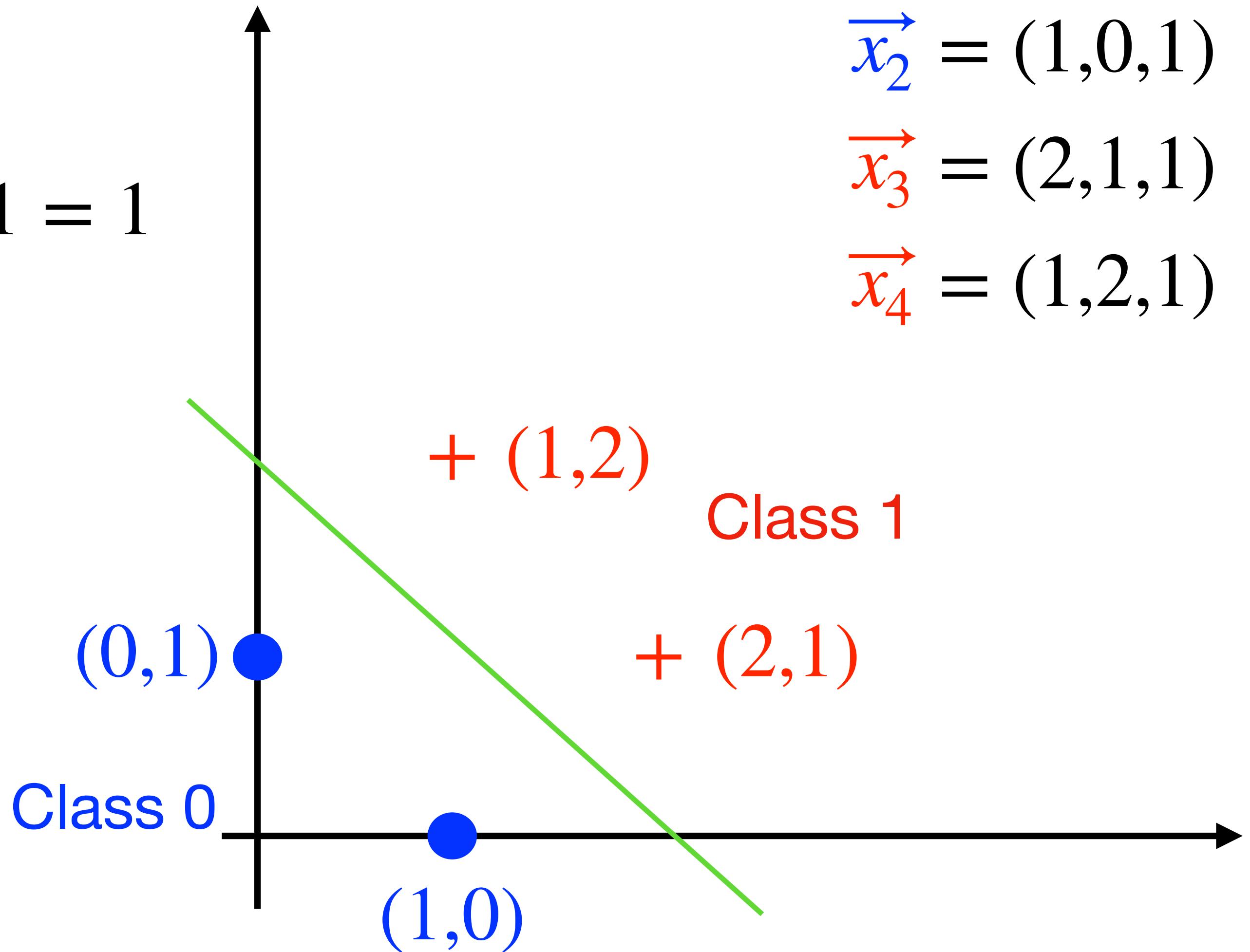
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$$\vec{x}_2 : \langle \vec{w}, \vec{x}_2 \rangle = -1$$

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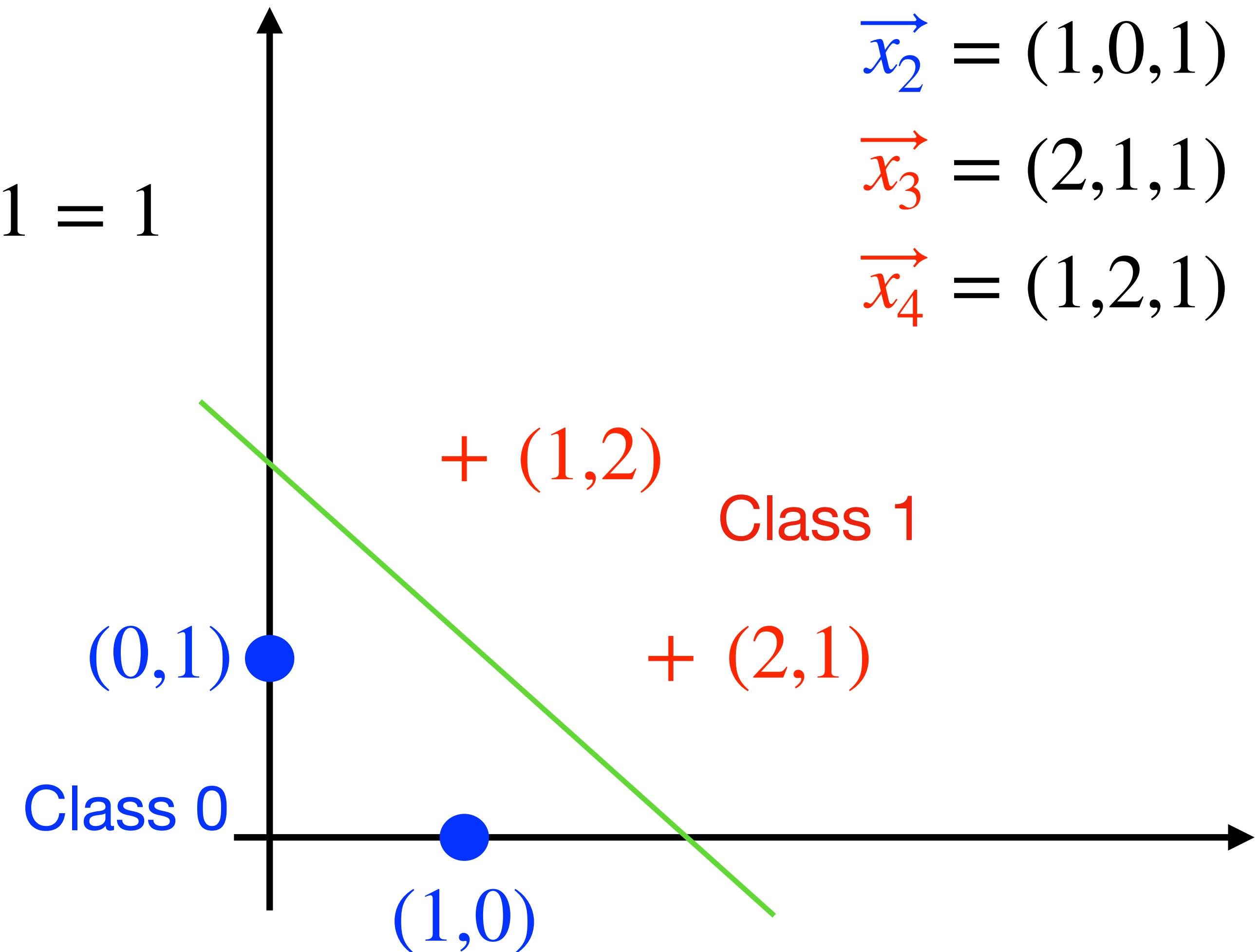
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correct prediction, no update



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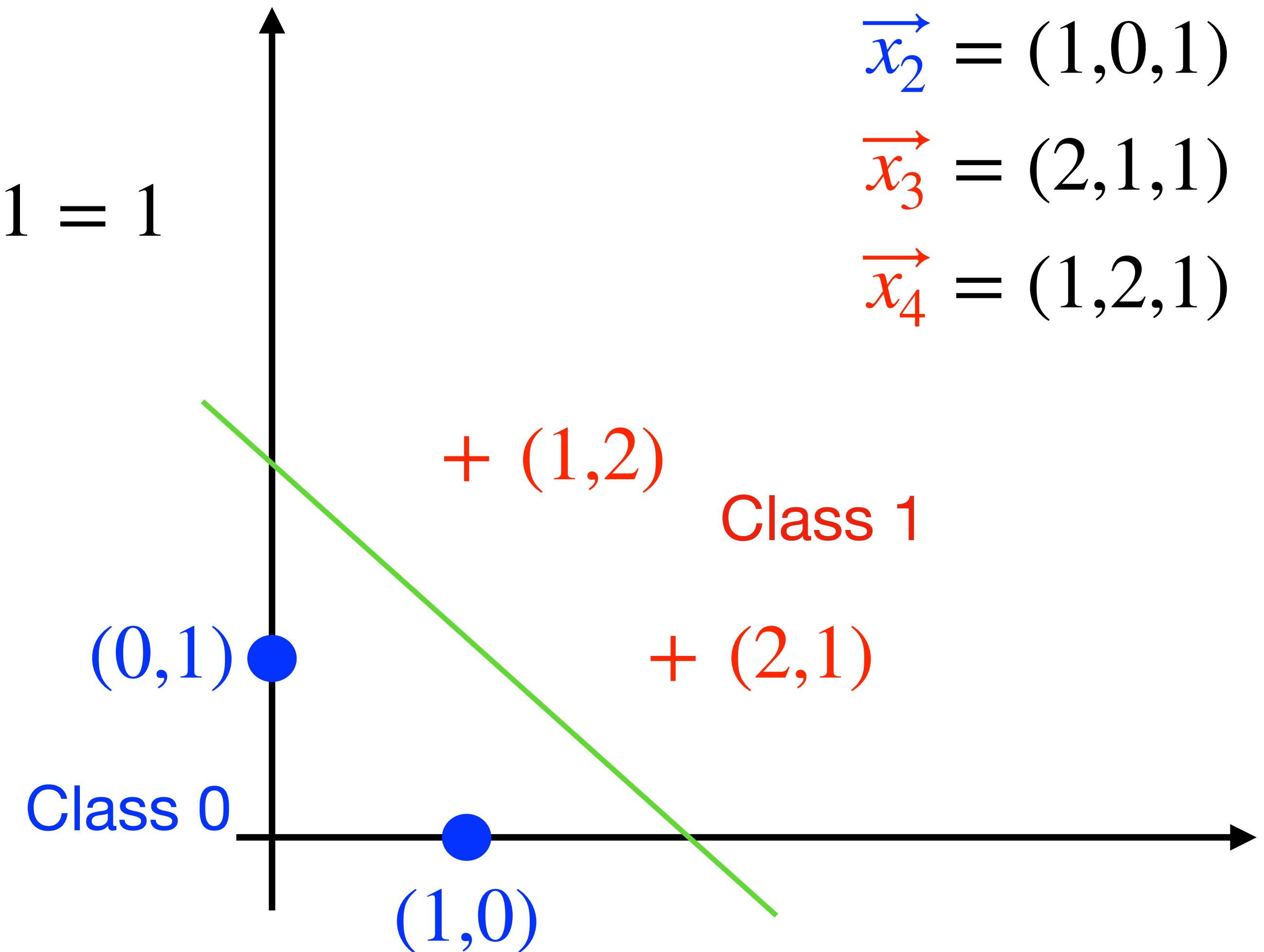
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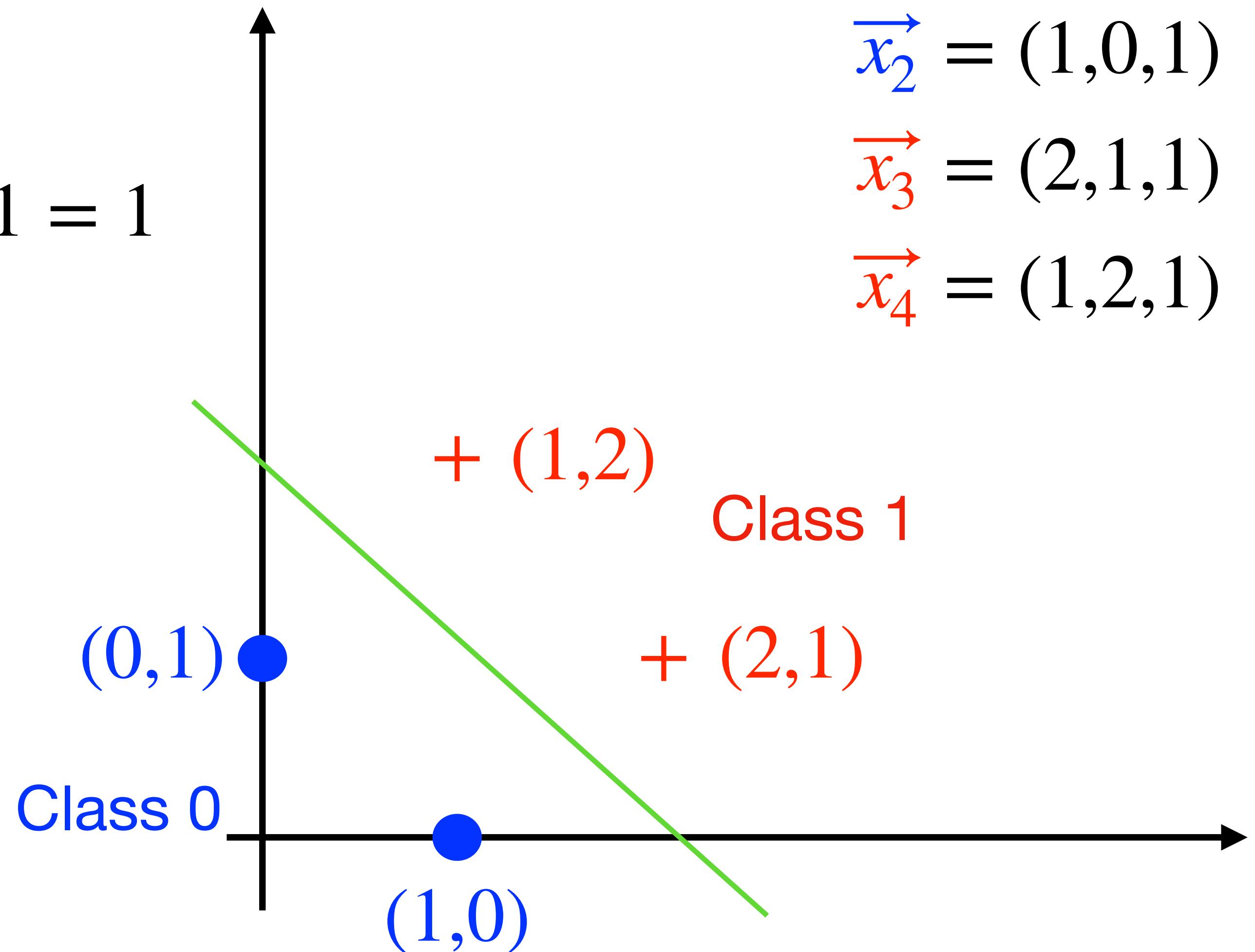
$$\vec{x}_3 : \langle \vec{w}, \vec{x}_3 \rangle = 1$$

correct prediction, no update

$$\vec{x}_4 : \langle \vec{w}, \vec{x}_4 \rangle = 1$$

correct prediction, no update

$$\begin{aligned}\vec{w} &= (1, 1, -2) \\ \vec{x}_1 &= (0, 1, 1) \\ \vec{x}_2 &= (1, 0, 1) \\ \vec{x}_3 &= (2, 1, 1) \\ \vec{x}_4 &= (1, 2, 1)\end{aligned}$$



Example: Training the Perceptron

- Second Epoch:

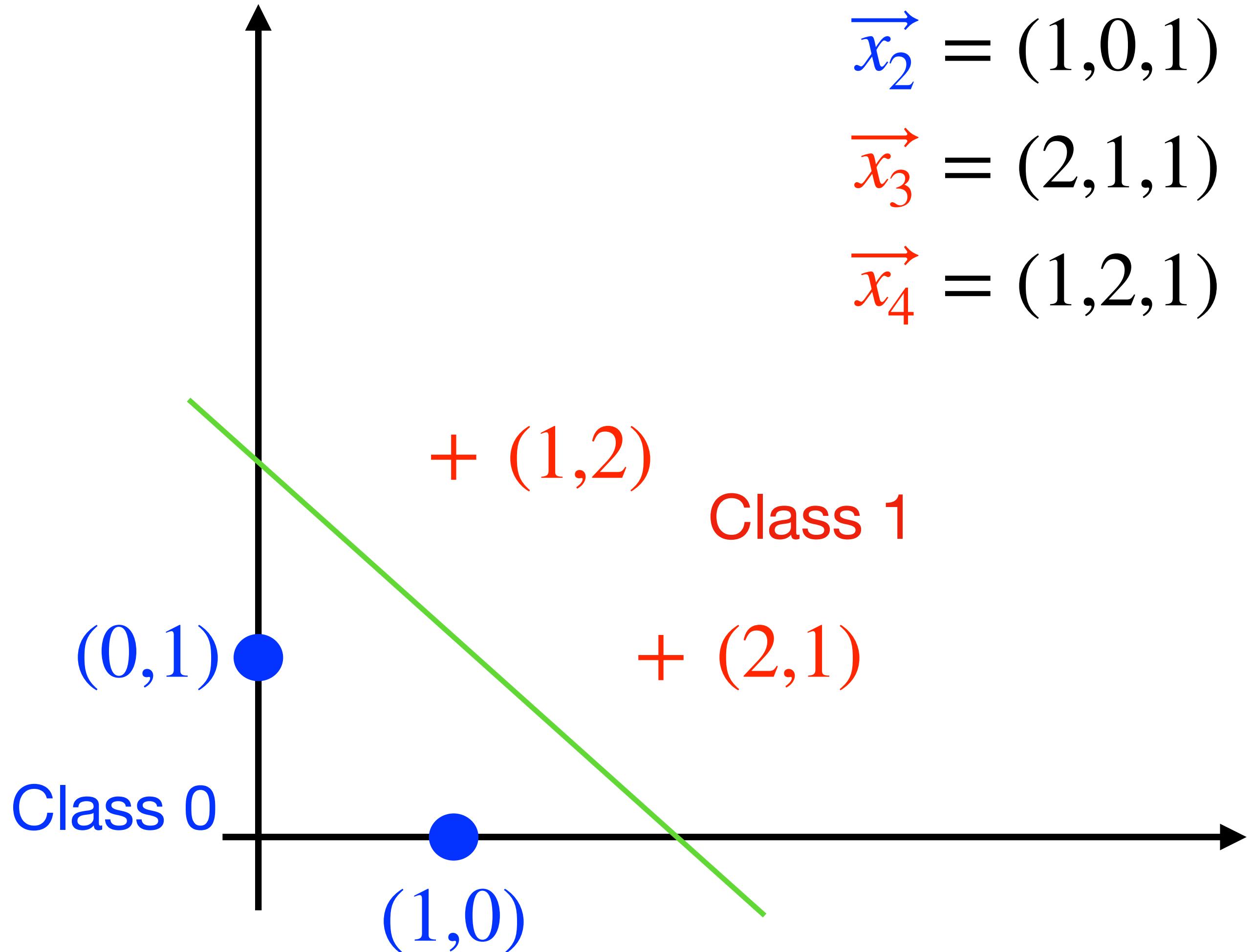
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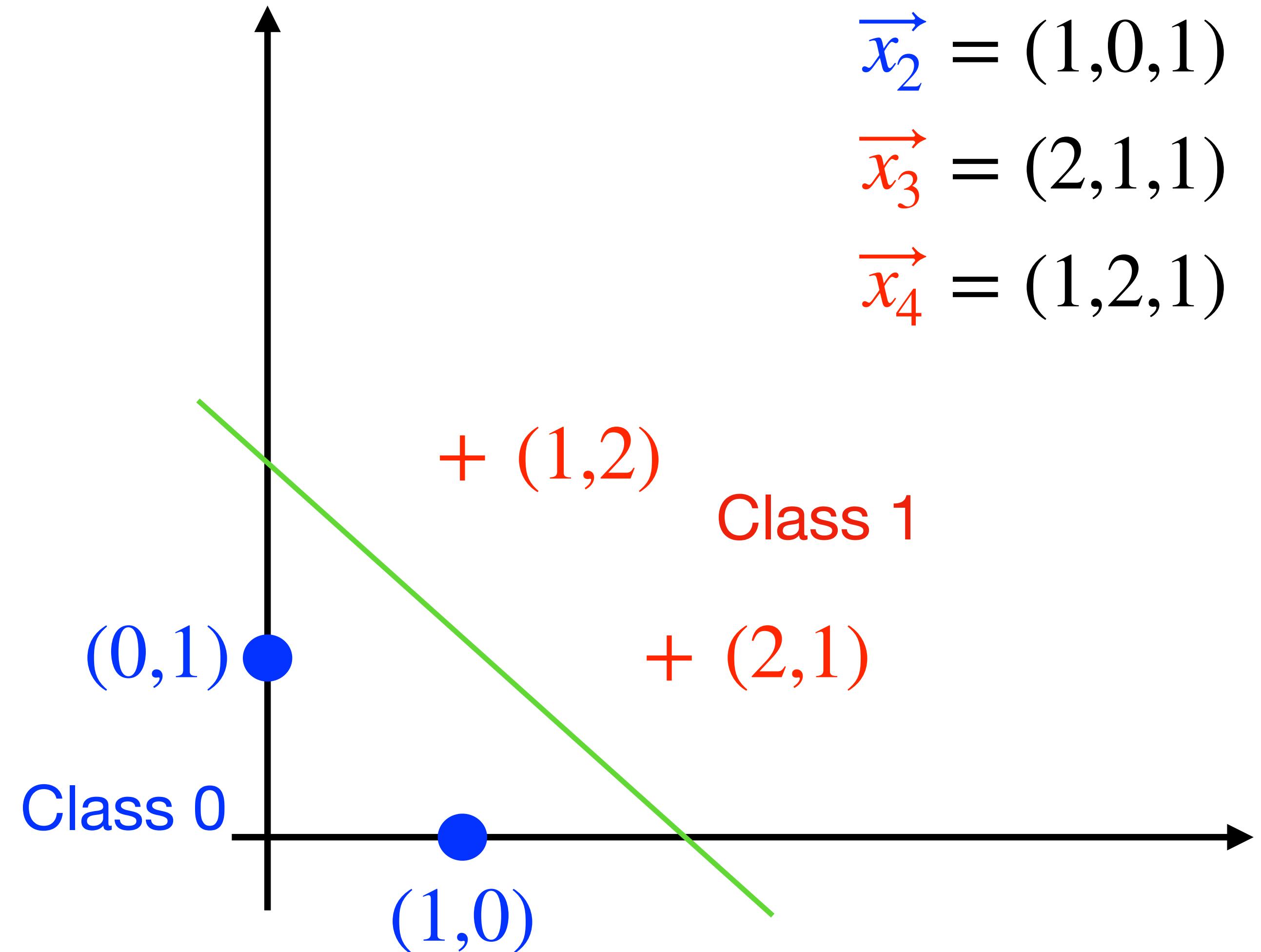
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$$\vec{x}_4 : \langle \vec{w}, \vec{x}_4 \rangle = 1, \quad \text{correct}$$

- Success!



$$\vec{w} = (1, 1, -2)$$

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Limitation: XOR Problem (Minsky & Papert, 1969)

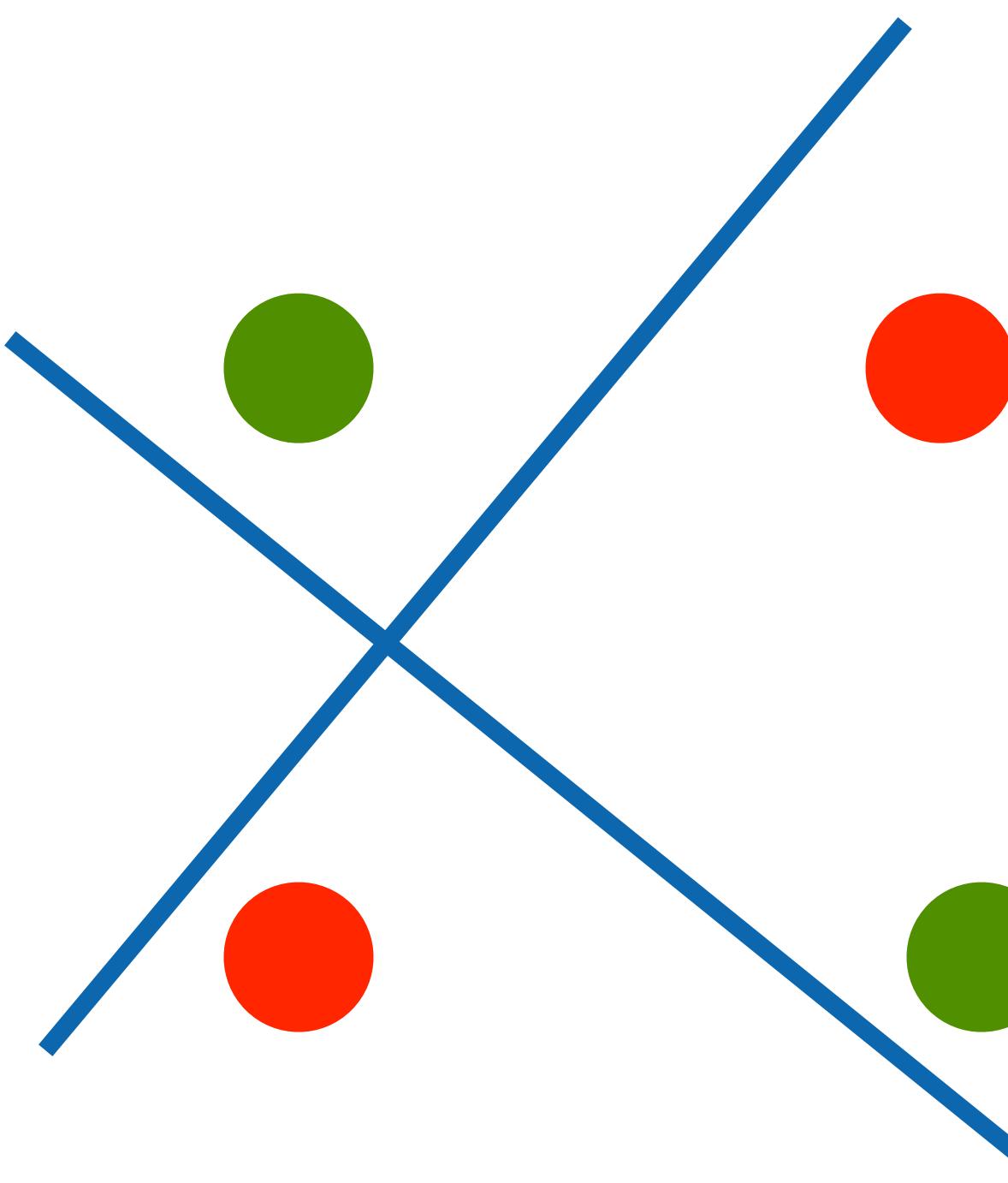
The perceptron cannot learn an XOR function
(neurons can only generate linear separators)

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

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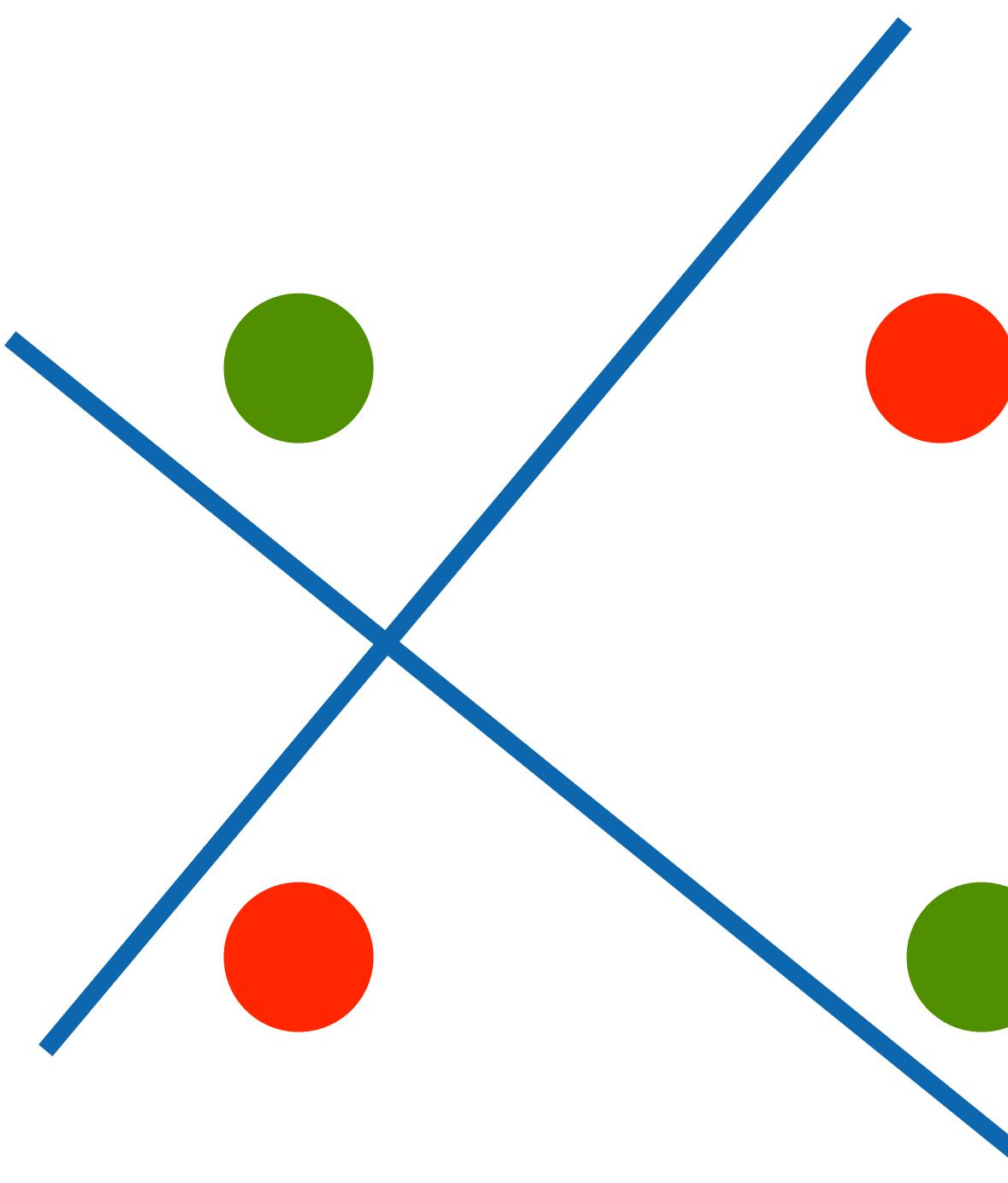
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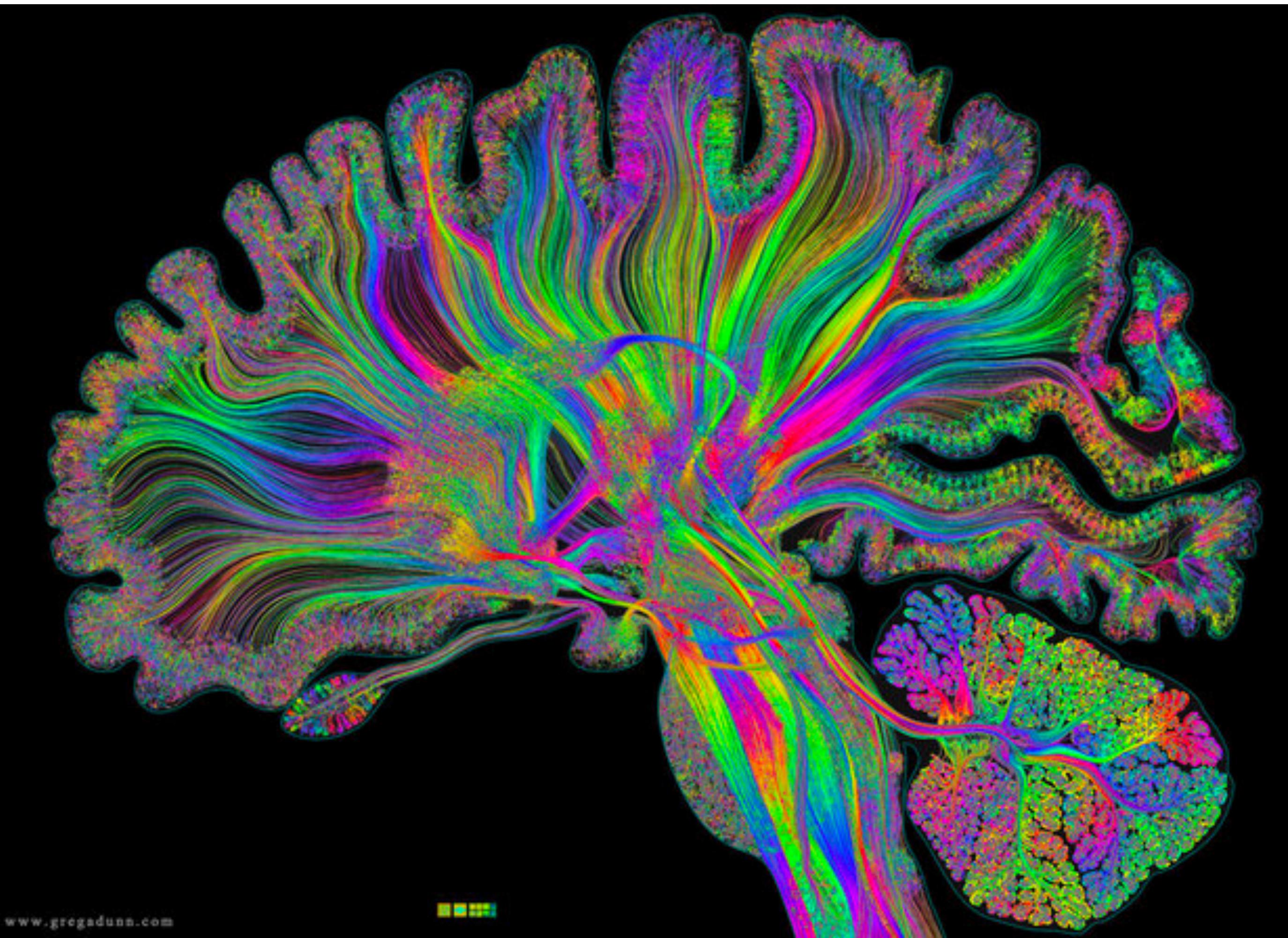
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On the other hand, perceptron can represent AND OR NOT, and their composition can represent all logic functions

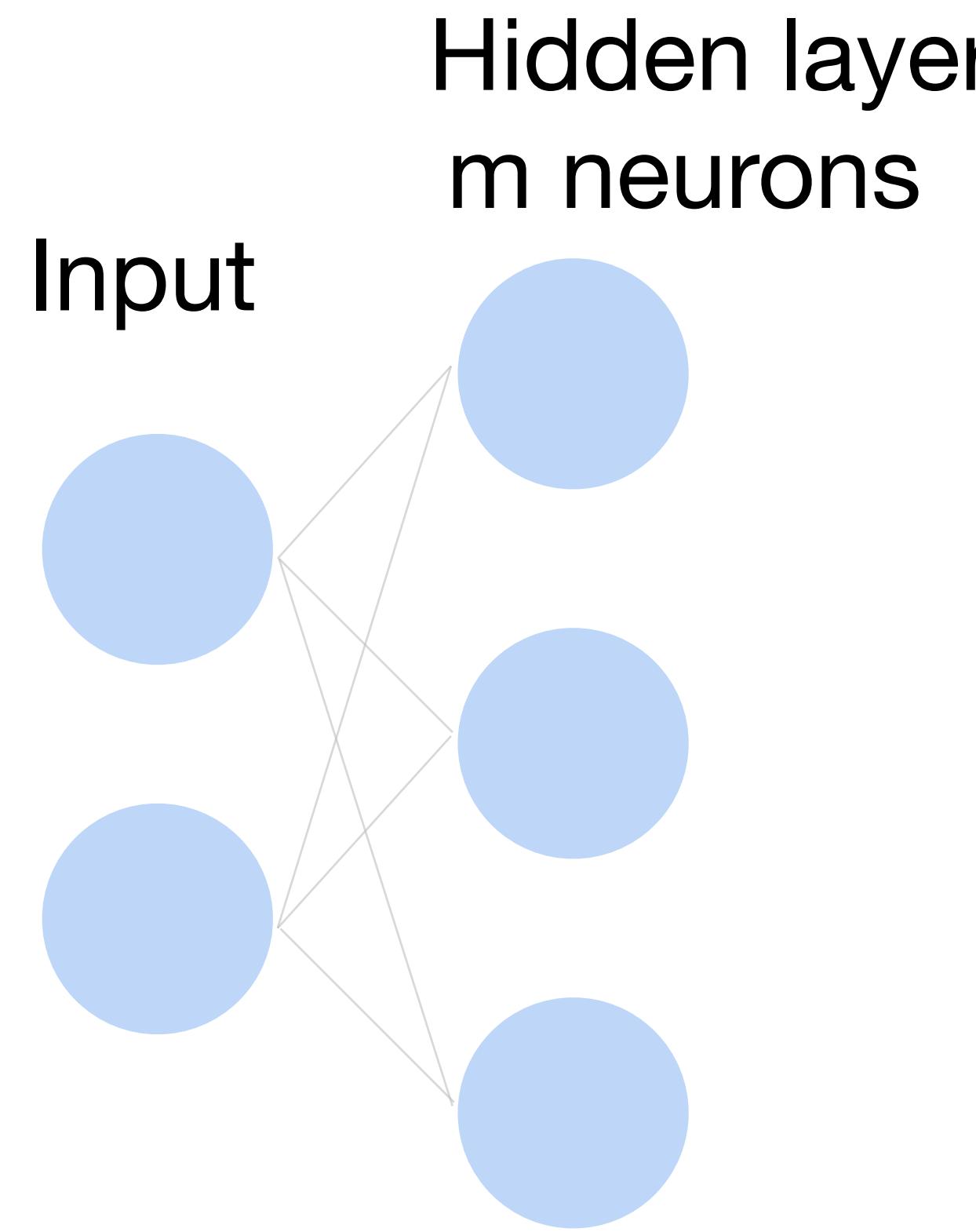
Multilayer Perceptron



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

σ is an element-wise activation function



Neural networks with one hidden layer

Key elements: linear operations + nonlinear activations

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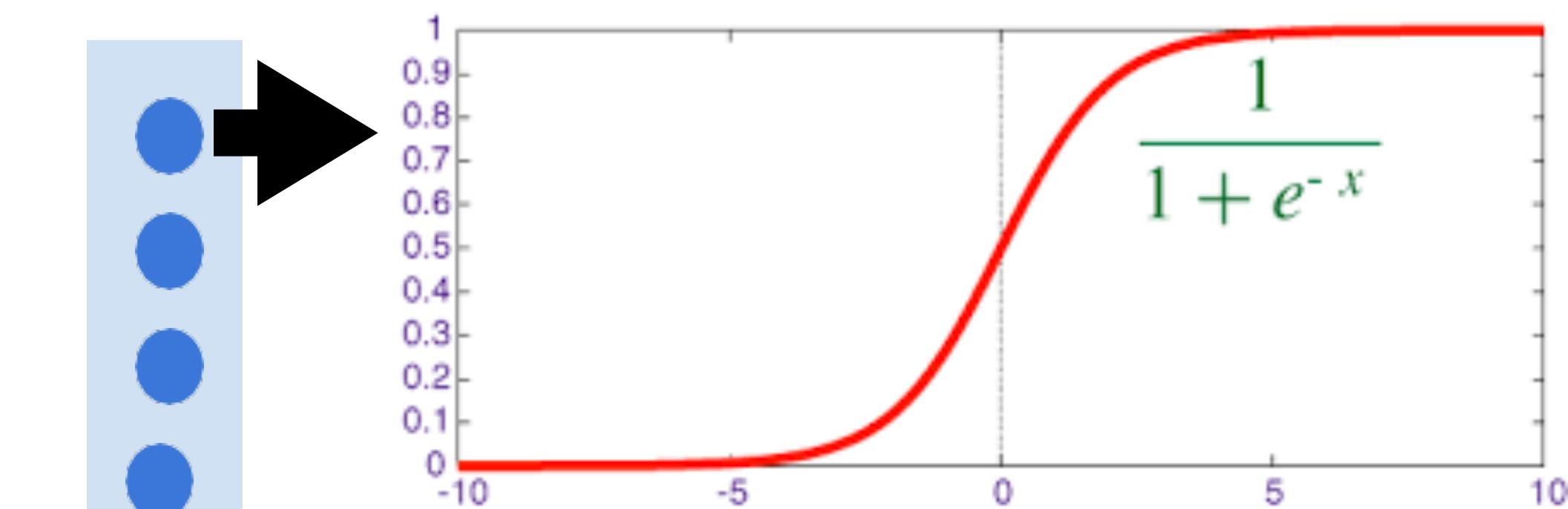
$$\begin{matrix} m \times d & & m \times 1 & & m \times 1 \\ \text{W} & \xrightarrow{\quad d \times 1 \quad} & \text{x} \in \mathbb{R}^d & + & \text{b} \\ \left[\begin{array}{c} \text{---} \\ \text{---} \end{array} \right] & & \left[\begin{array}{c} \text{---} \\ \text{---} \end{array} \right] & & \left[\begin{array}{c} \text{---} \\ \text{---} \end{array} \right] \end{matrix}$$

The diagram illustrates the computation of a neural network layer. It shows the multiplication of a weight matrix \mathbf{W} (dimensions $m \times d$) by an input vector $\mathbf{x} \in \mathbb{R}^d$ (dimensions $d \times 1$). The result is a vector \mathbf{b} (dimensions $m \times 1$) which is then added to a bias vector (dimensions $m \times 1$). The final output is a vector of m values, each represented by a blue circle.

Neural networks with one hidden layer

Key elements: linear operations + nonlinear activations

$$\begin{matrix} m \times d & & m \times 1 & & m \times 1 \\ \text{W} & \xrightarrow{\quad d \times 1 \quad} & \text{x} \in \mathbb{R}^d & + & \text{b} \end{matrix} =$$

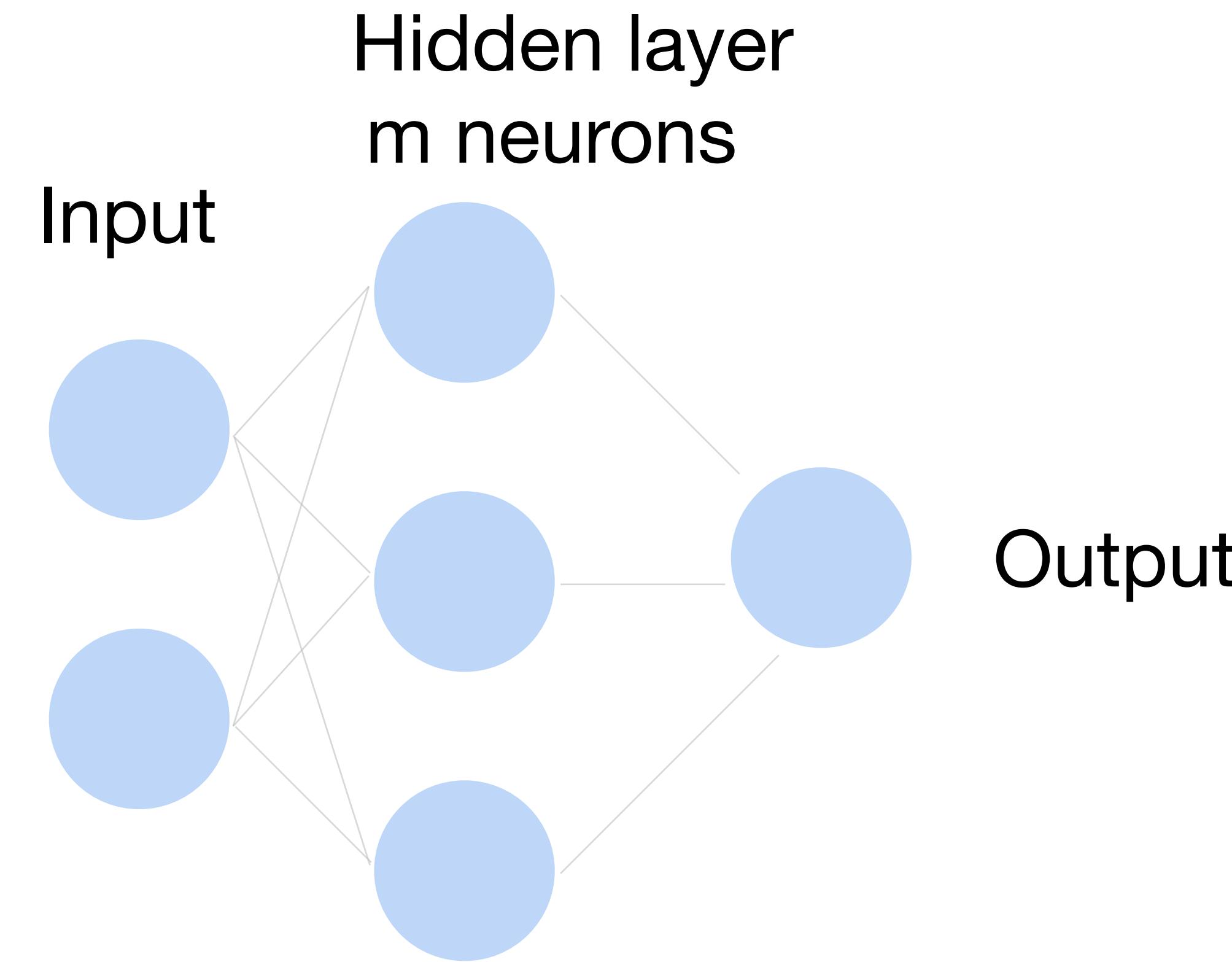
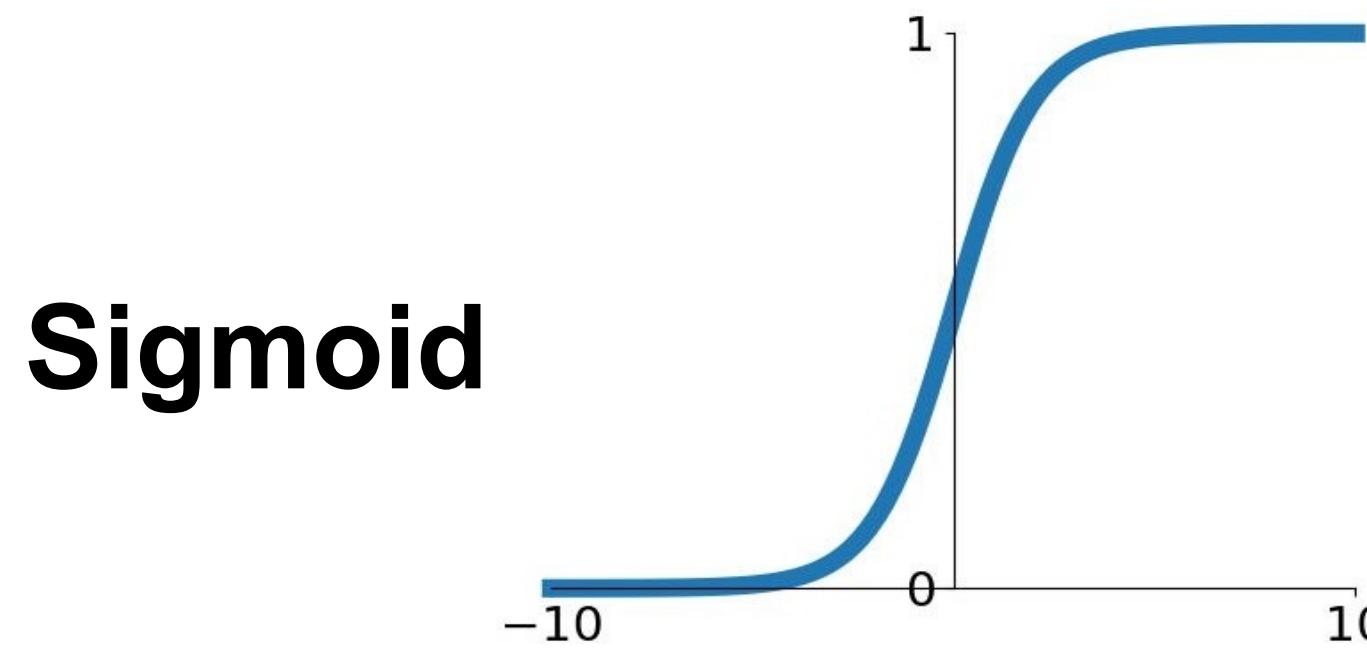


Element-wise
activation function

Single Hidden Layer

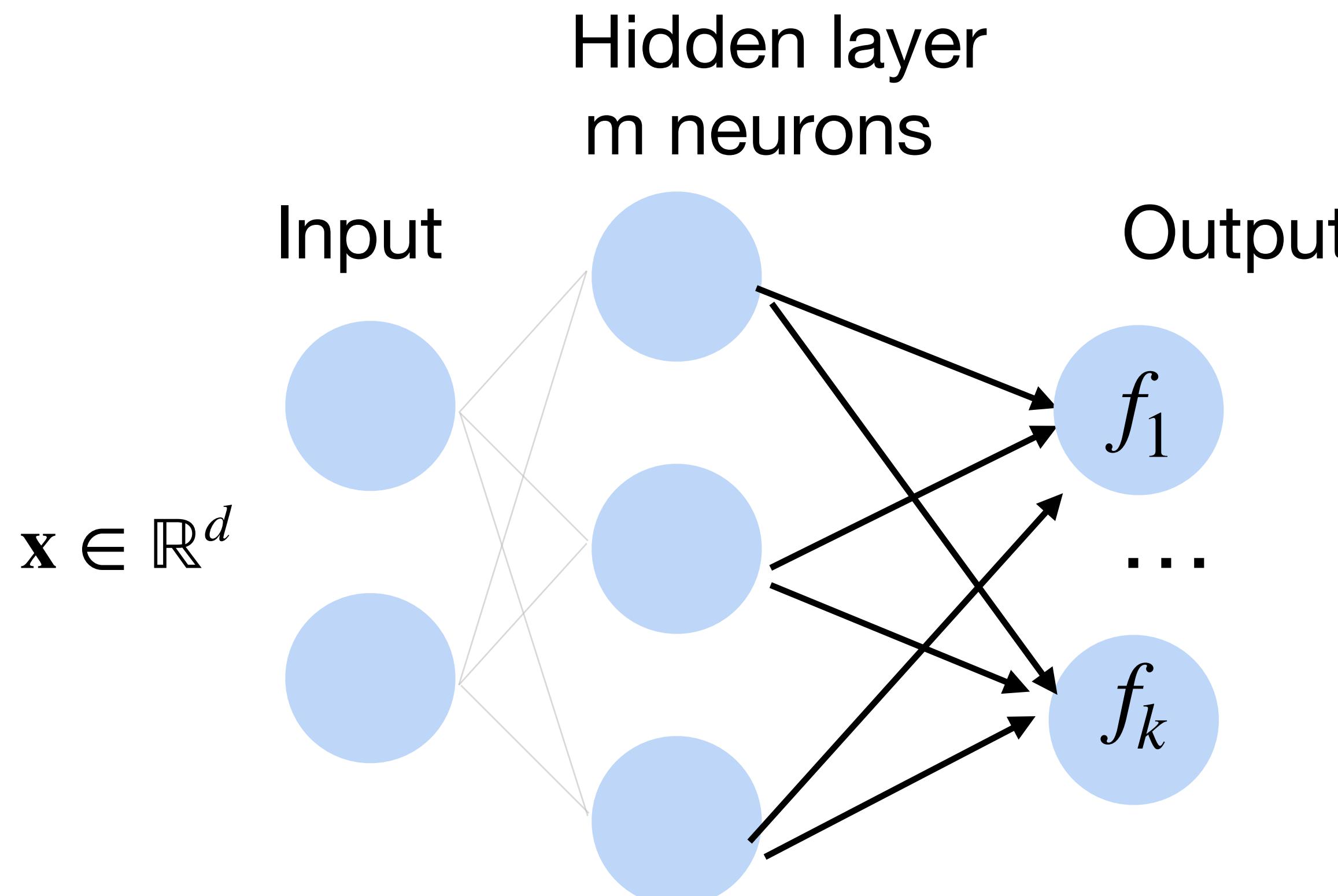
- Output $f = \mathbf{w}_2^\top \mathbf{h} + b_2$
- Normalize the output into probability using sigmoid

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



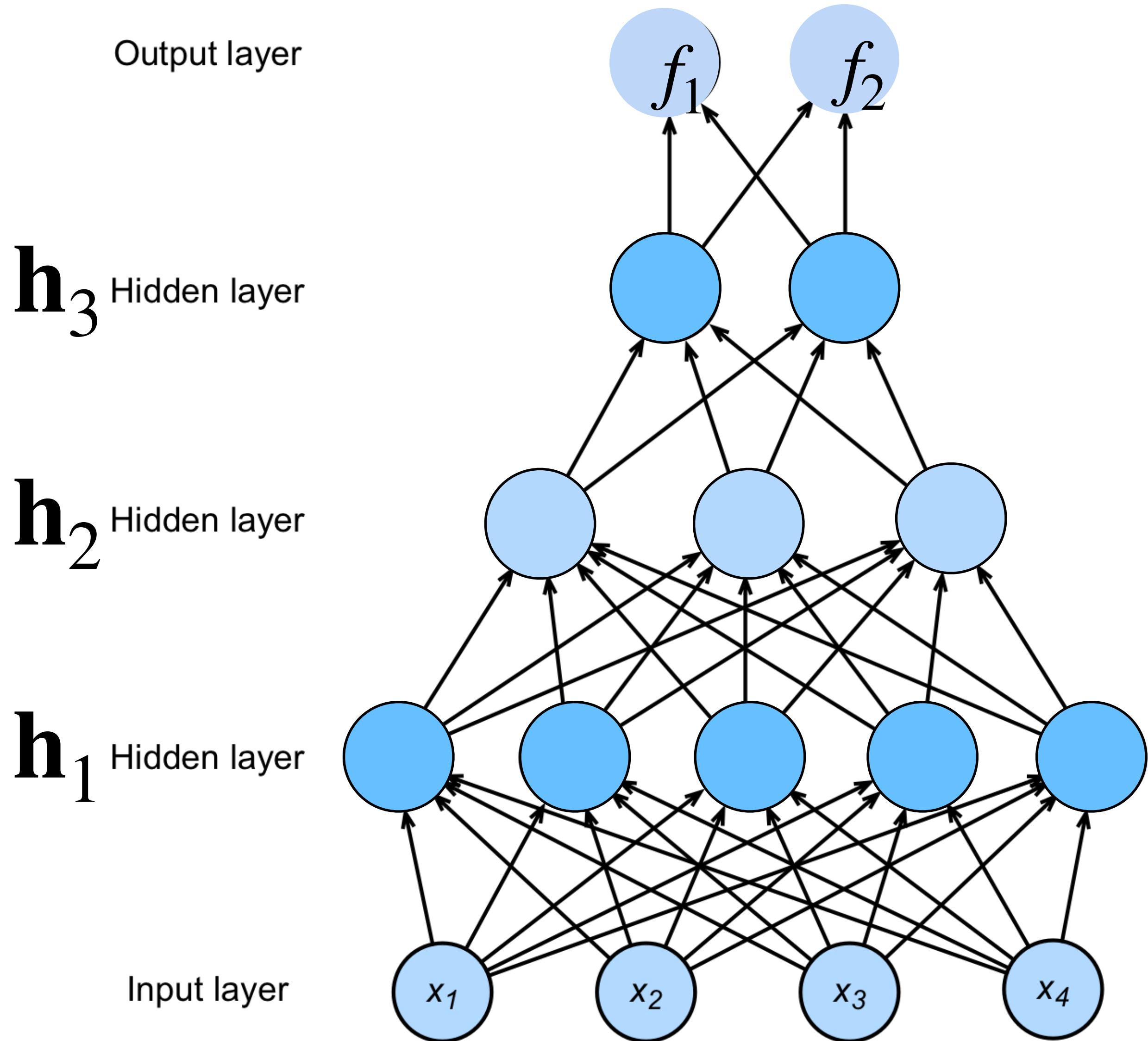
Multi-class classification

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



$$p(y | x) = \text{softmax}(f)$$
$$= \frac{\exp f_y(x)}{\sum_i^k \exp f_i(x)}$$

Deep neural networks (DNNs)



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

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

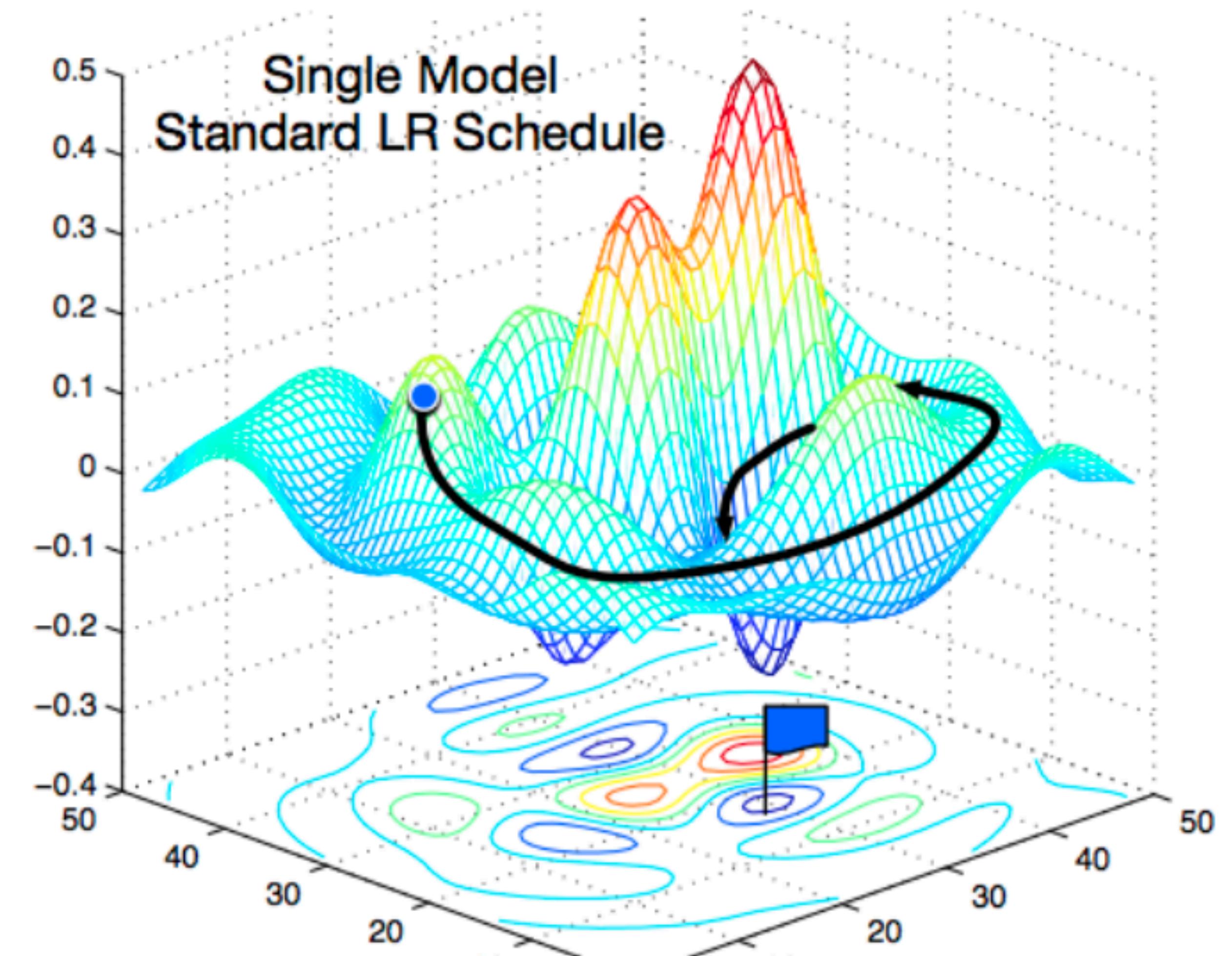
$$\mathbf{h}_3 = \sigma(\mathbf{W}_3 \mathbf{h}_2 + \mathbf{b}_3)$$

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

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

NNs are composition
of nonlinear
functions

Training Neural Networks



[Gao and Li et al., 2018]

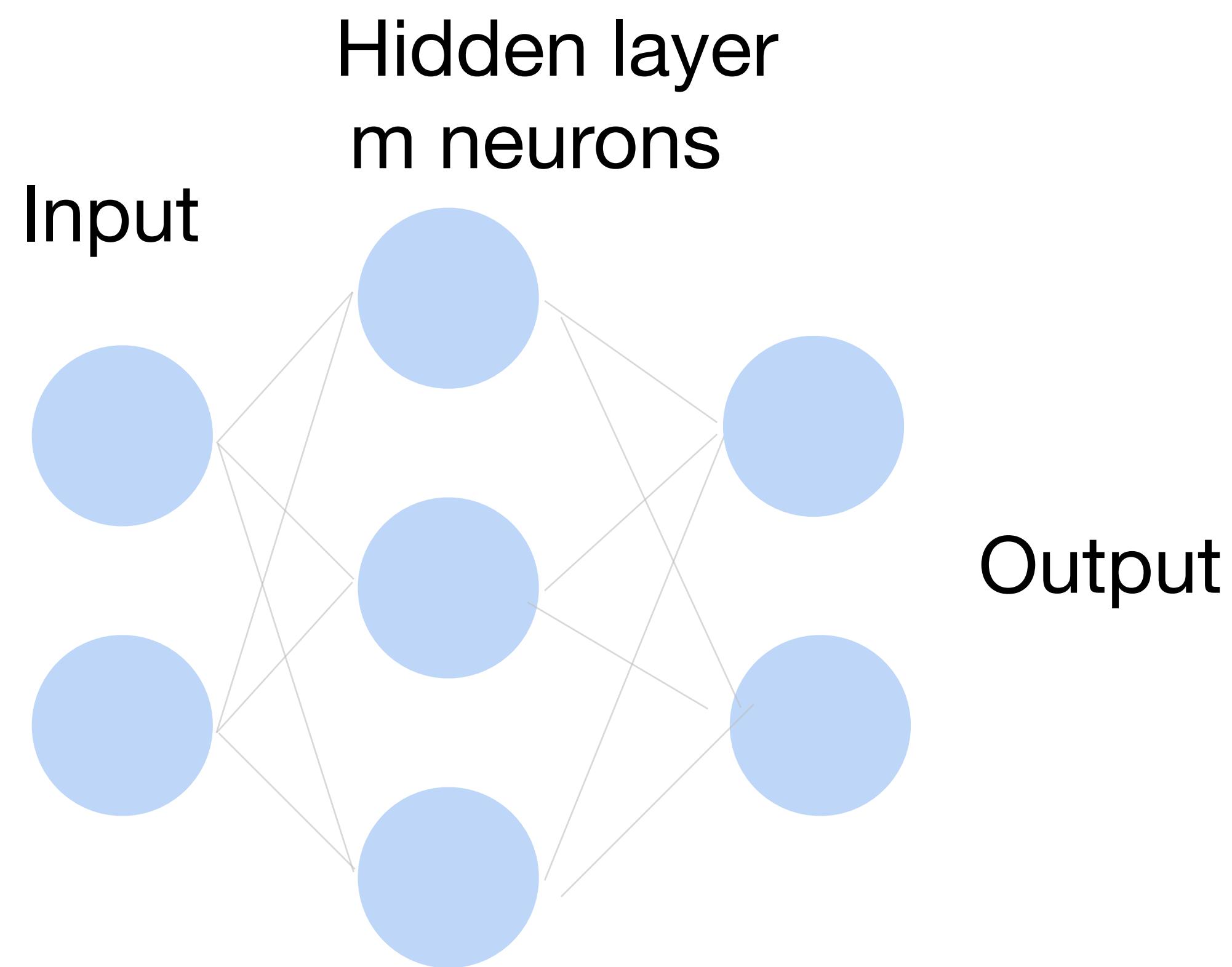
Cross-Entropy Loss

Loss: $\frac{1}{|D|} \sum_{(\mathbf{x}, y) \in D} \ell(\mathbf{x}, y)$

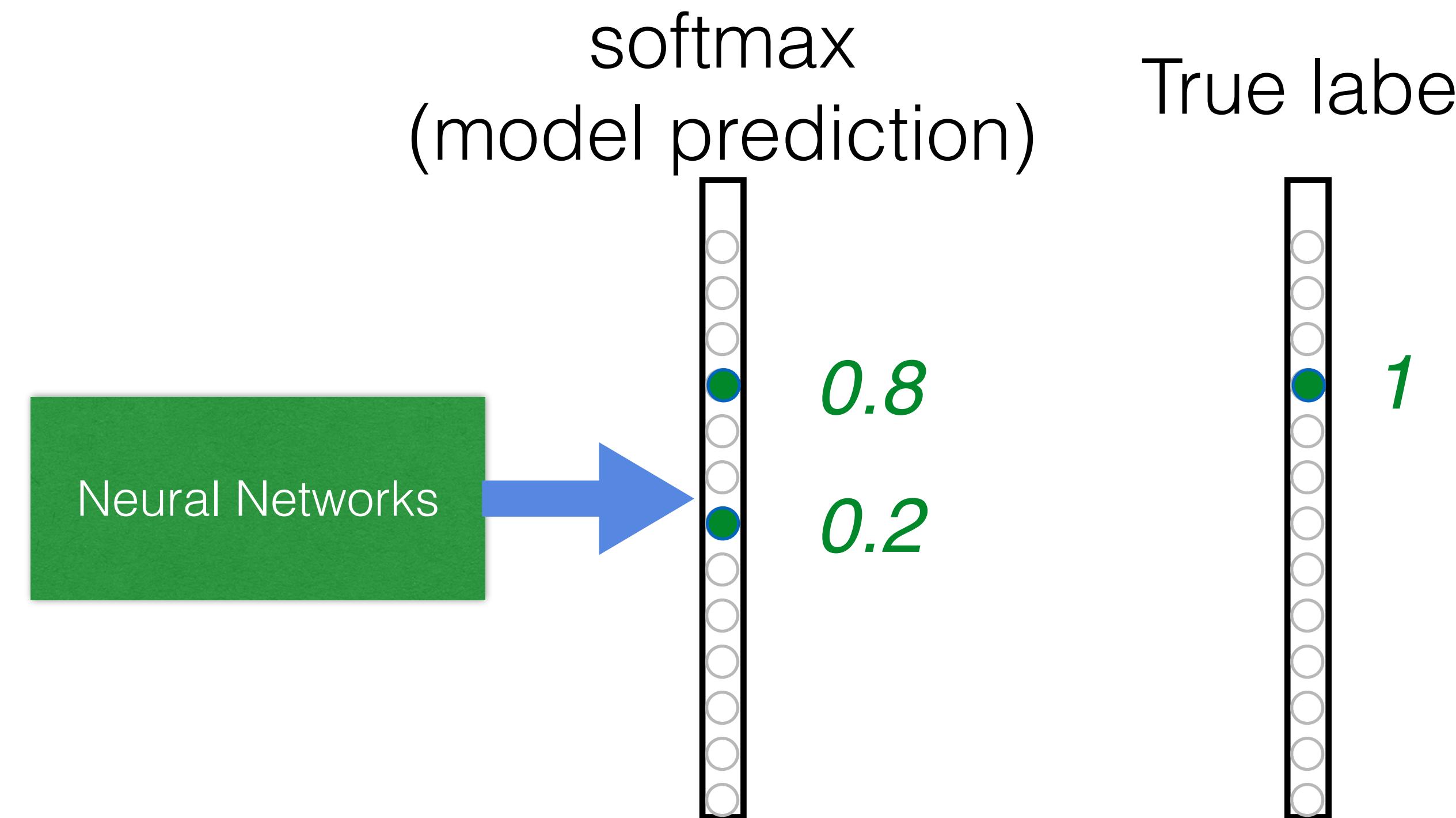
Per sample loss (cross-entropy or softmax loss):

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

where Y is one-hot encoding of y



Cross-Entropy Loss



$$\begin{aligned} L_{CE} &= \sum_j -Y_j \log(p_j) \\ &= -\log(0.8) \end{aligned}$$

Goal: push \mathbf{p} and \mathbf{Y} to be identical

Binary Cross-Entropy Loss

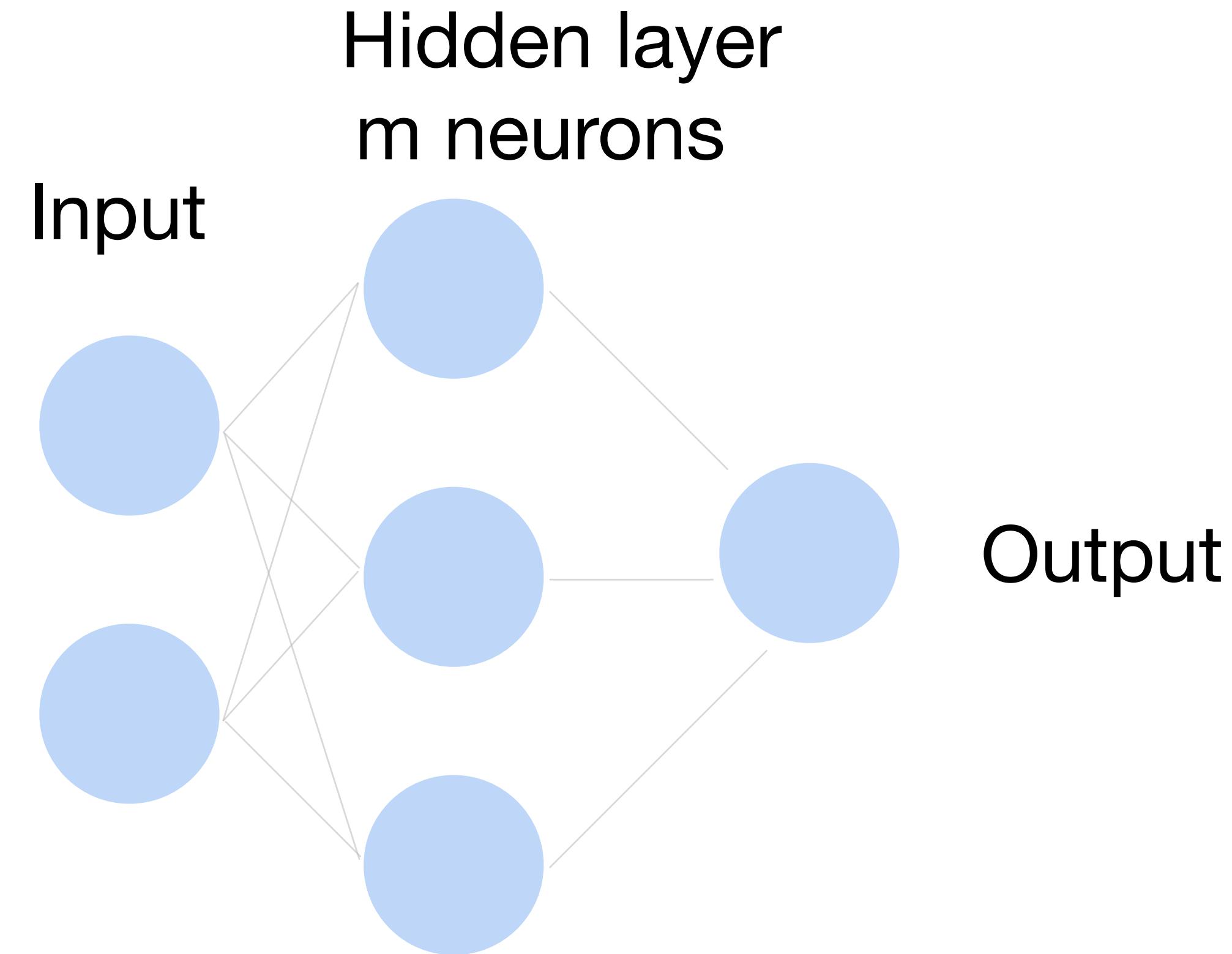
Loss: $\frac{1}{|D|} \sum_{(\mathbf{x}, y) \in D} \ell(\mathbf{x}, y)$

Binary cross-entropy loss can be viewed as a special case of cross-entropy loss:

$$\ell(\mathbf{x}, y) = -y \log p - (1 - y) \log(1 - p)$$

Think of the output as a probability vector ($p_0 = 1 - p, p_1 = p$) over the classes {0, 1}:

$$\ell(\mathbf{x}, y) = -\log p_y$$

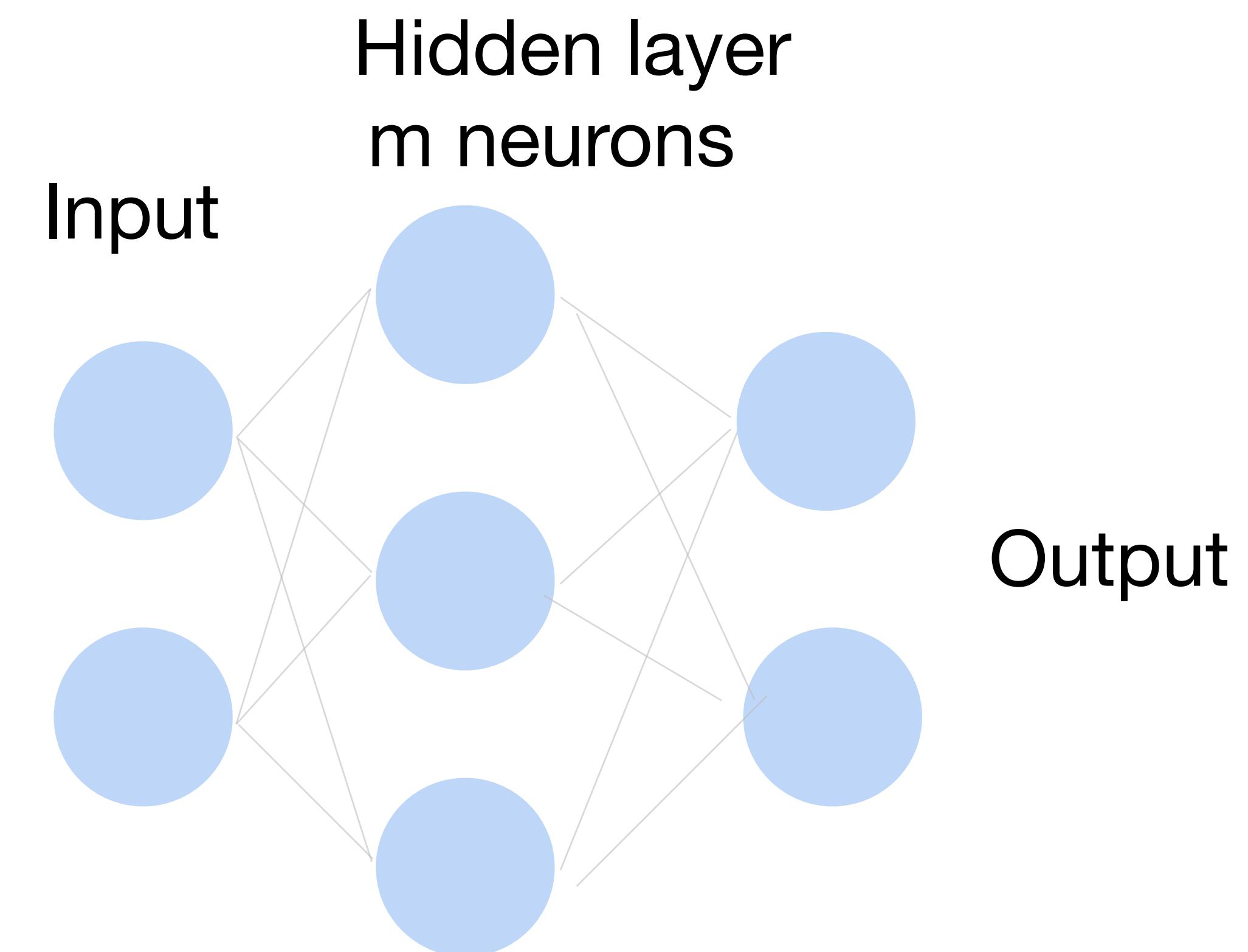


How to train a neural network?

Update the weights W to minimize the loss function

$$L = \frac{1}{|D|} \sum_{(\mathbf{x}, y) \in D} \ell(\mathbf{x}, y)$$

Use gradient descent!



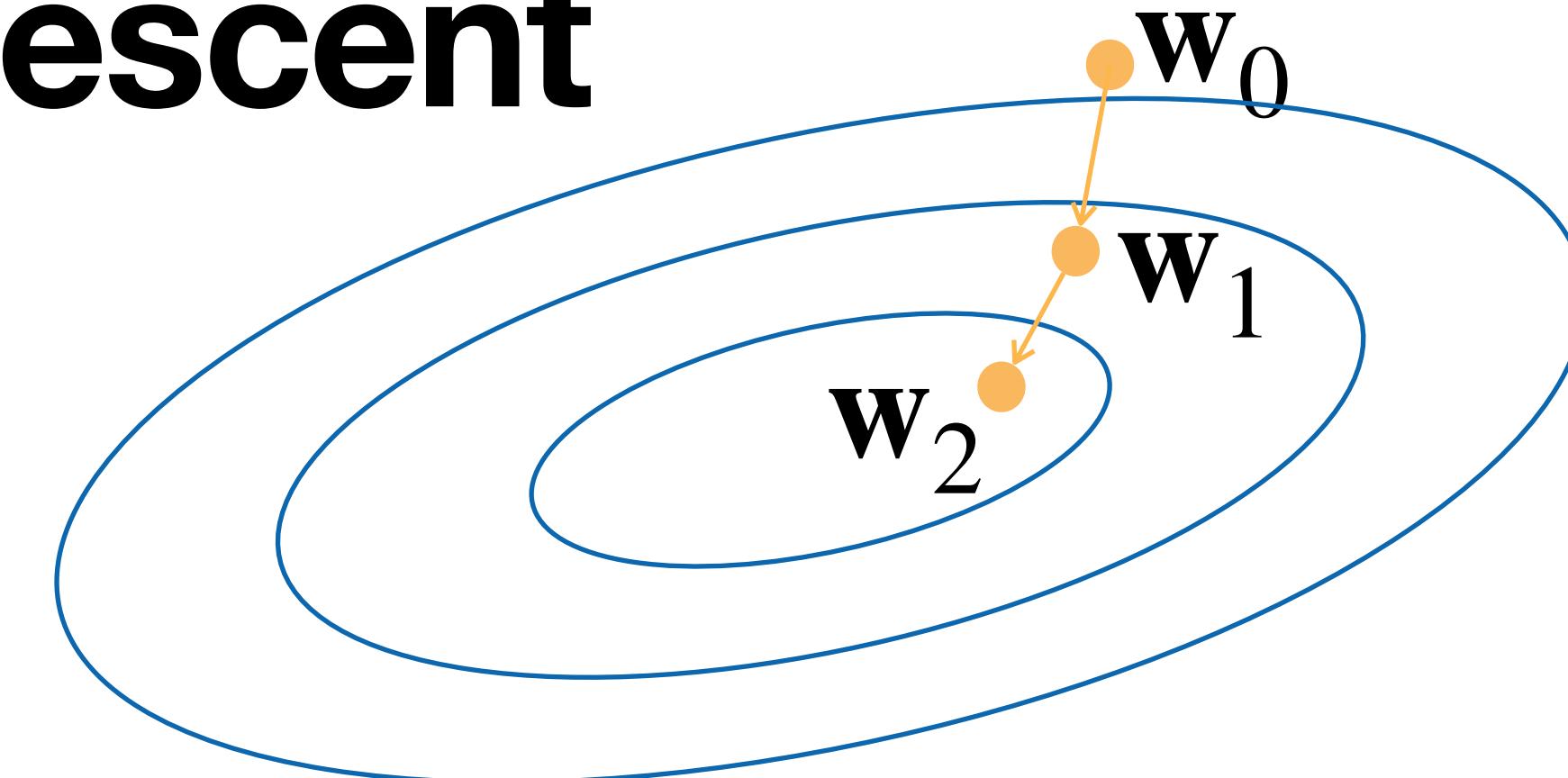
Minibatch Stochastic Gradient Descent

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

- 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



Minibatch Stochastic Gradient Descent

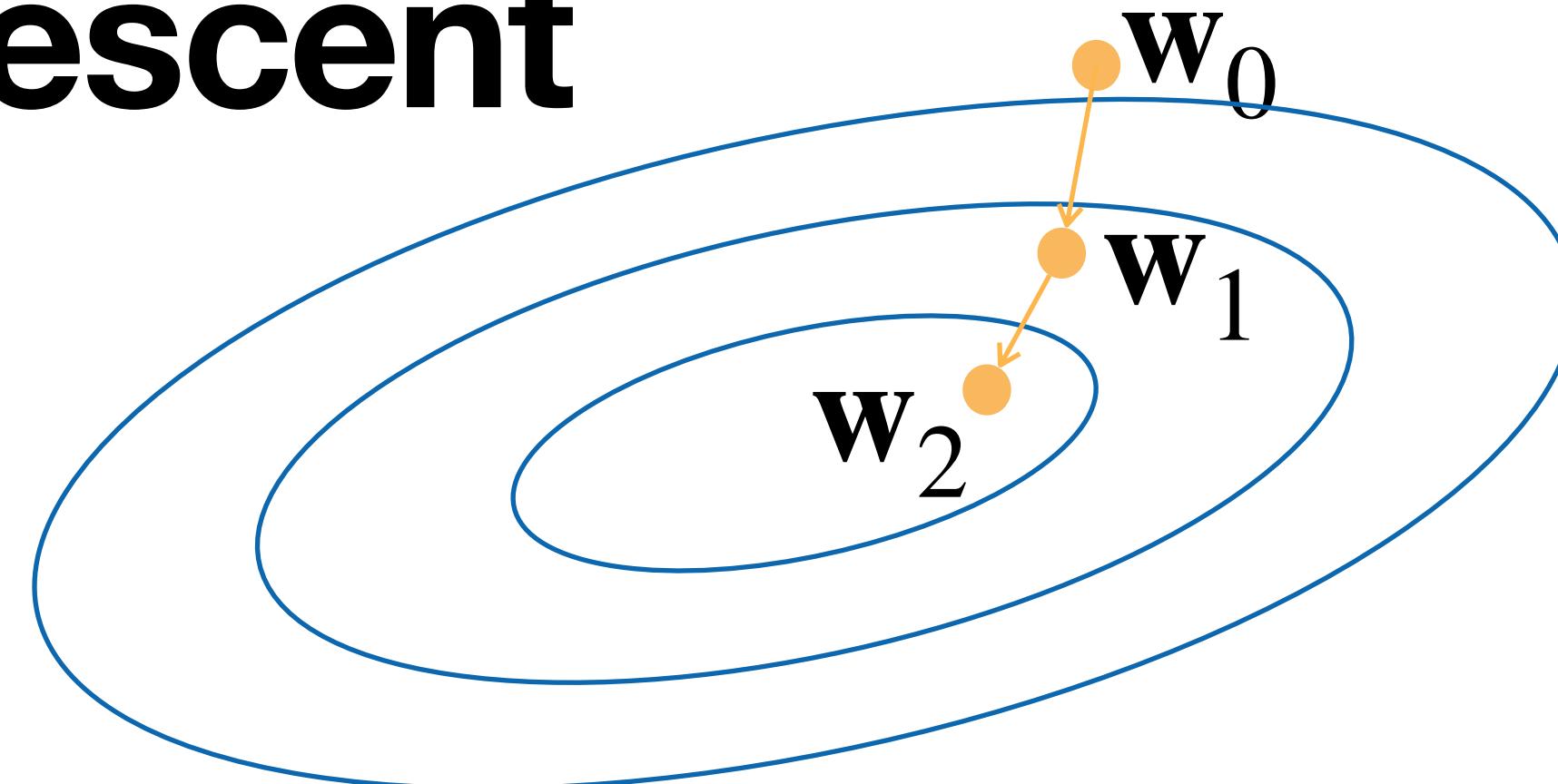
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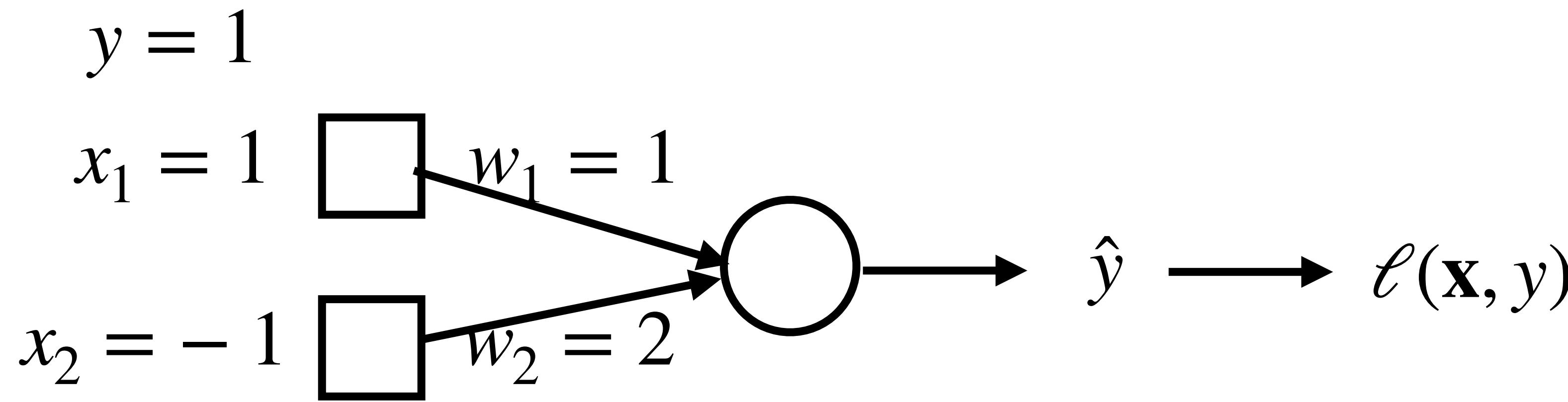
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The gradient w.r.t. all parameters is obtained by concatenating the partial derivatives w.r.t. each parameter

Example: Backpropagation

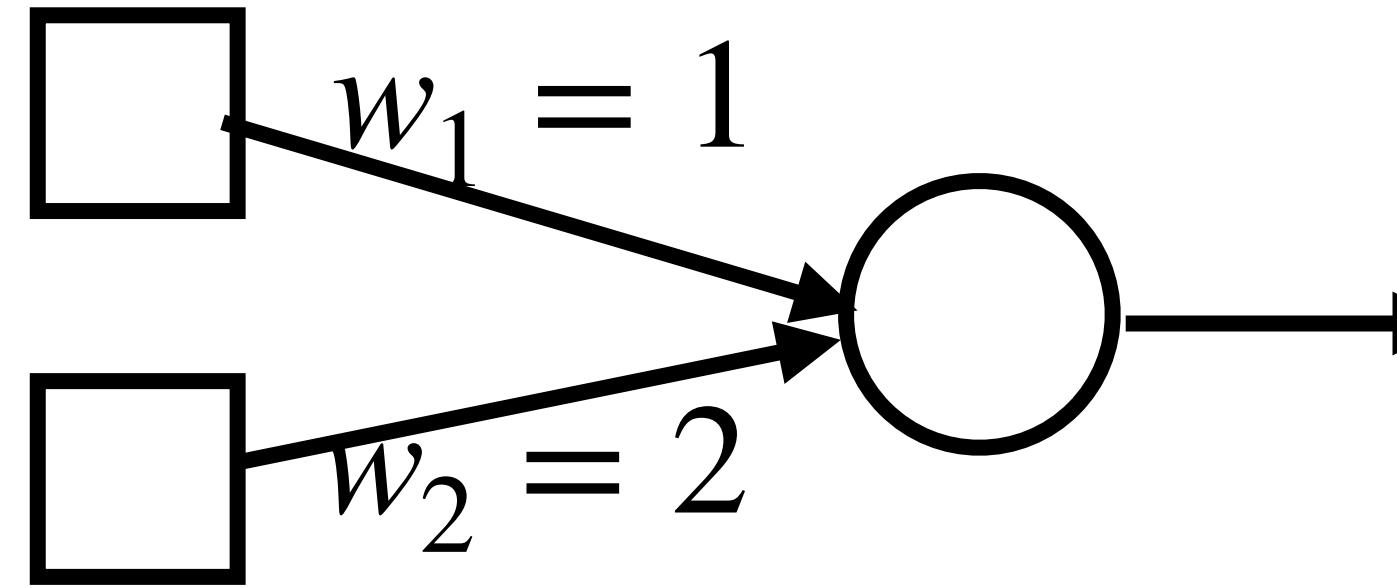


Example: Backpropagation

$$y = 1$$

$$x_1 = 1$$

$$x_2 = -1$$



sigmoid activation, binary cross-entropy loss

$$\hat{y} = \sigma(w_1x_1 + w_2x_2)$$

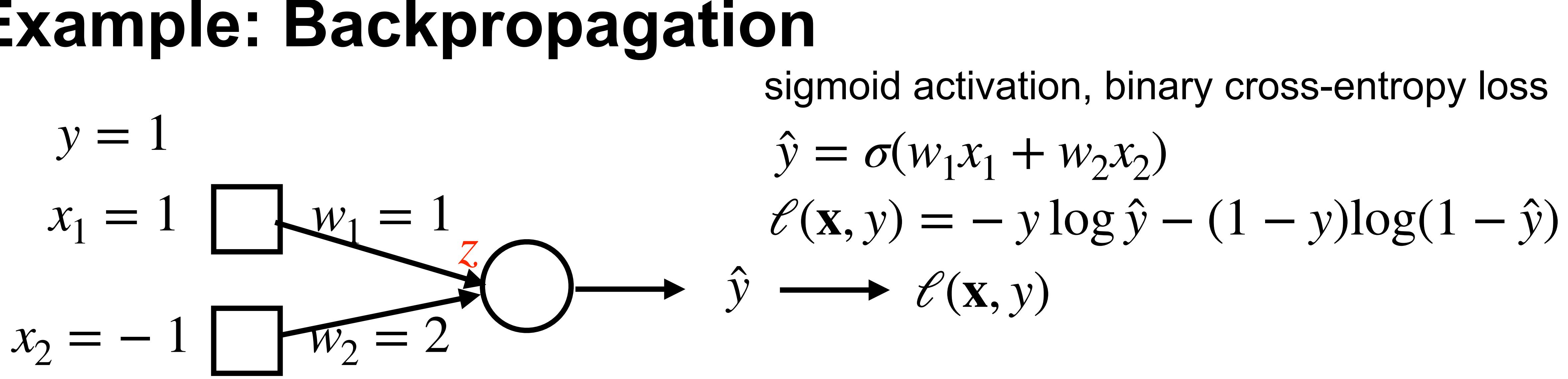
$$\ell(\mathbf{x}, y) = -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$$

$$\hat{y} \longrightarrow \ell(\mathbf{x}, y)$$

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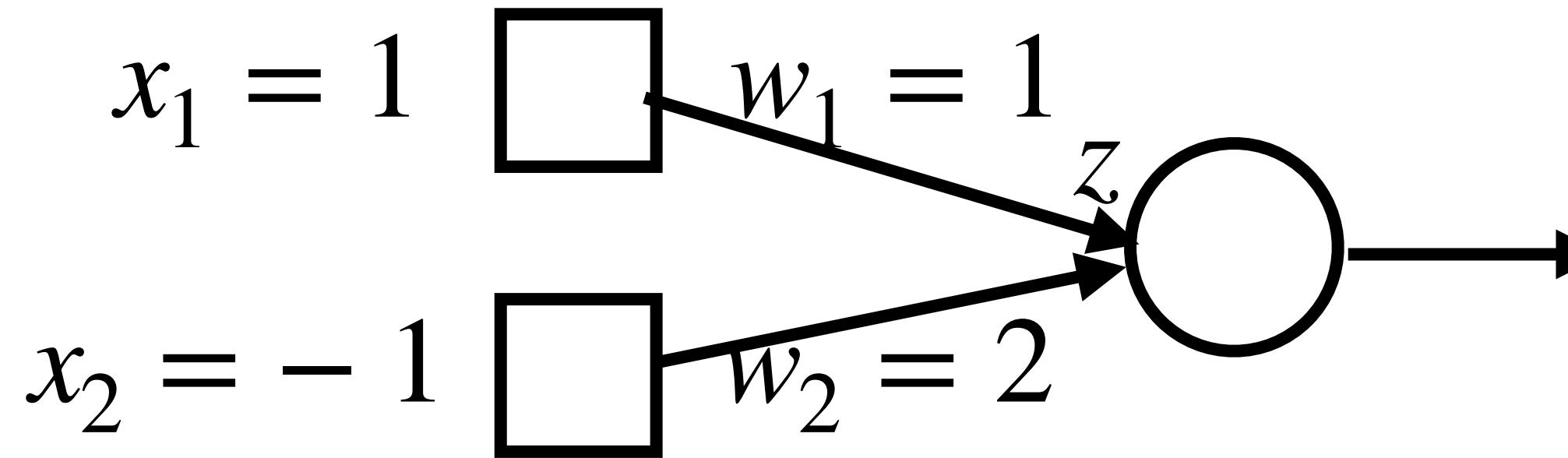
- Forward:

$$z = w_1x_1 + w_2x_2 = 1 \times 1 + (-1) \times 2 = -1$$

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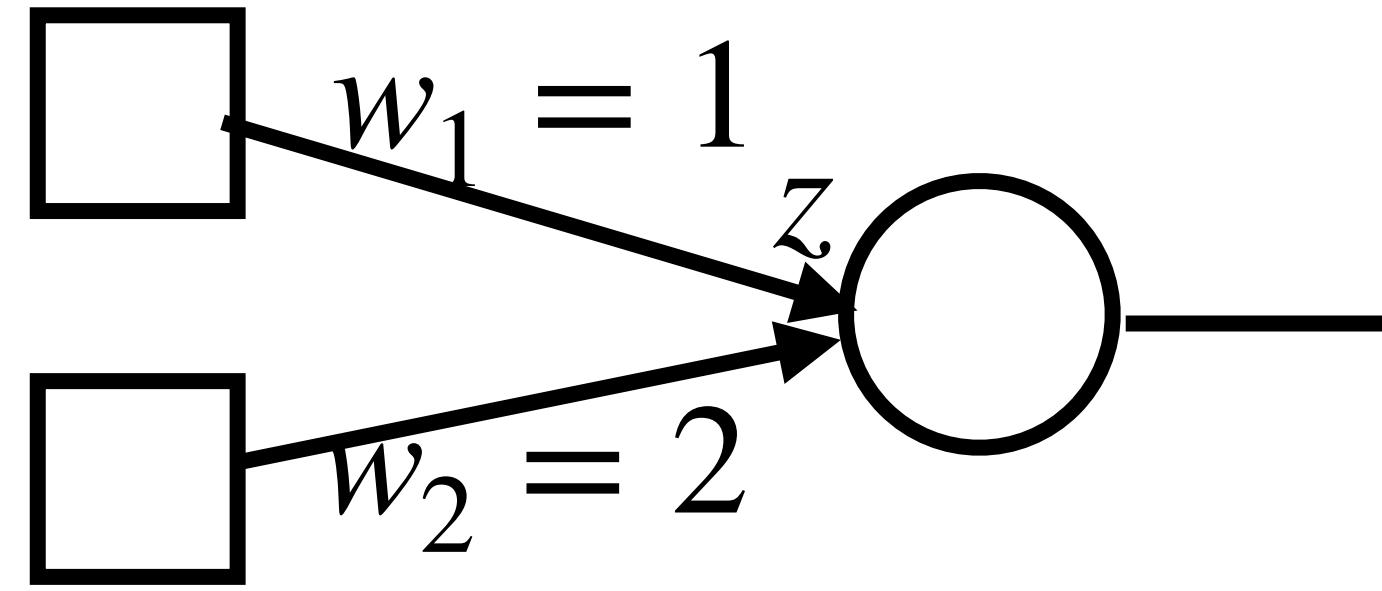
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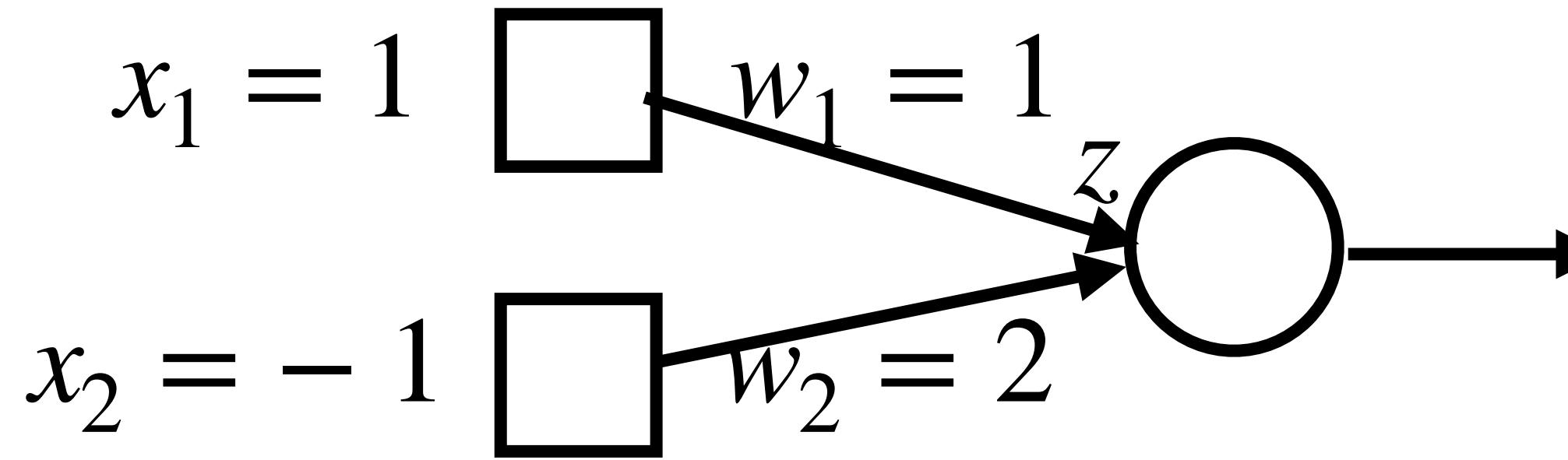
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$$\hat{y} \longrightarrow \ell(\mathbf{x}, y)$$

- Forward:

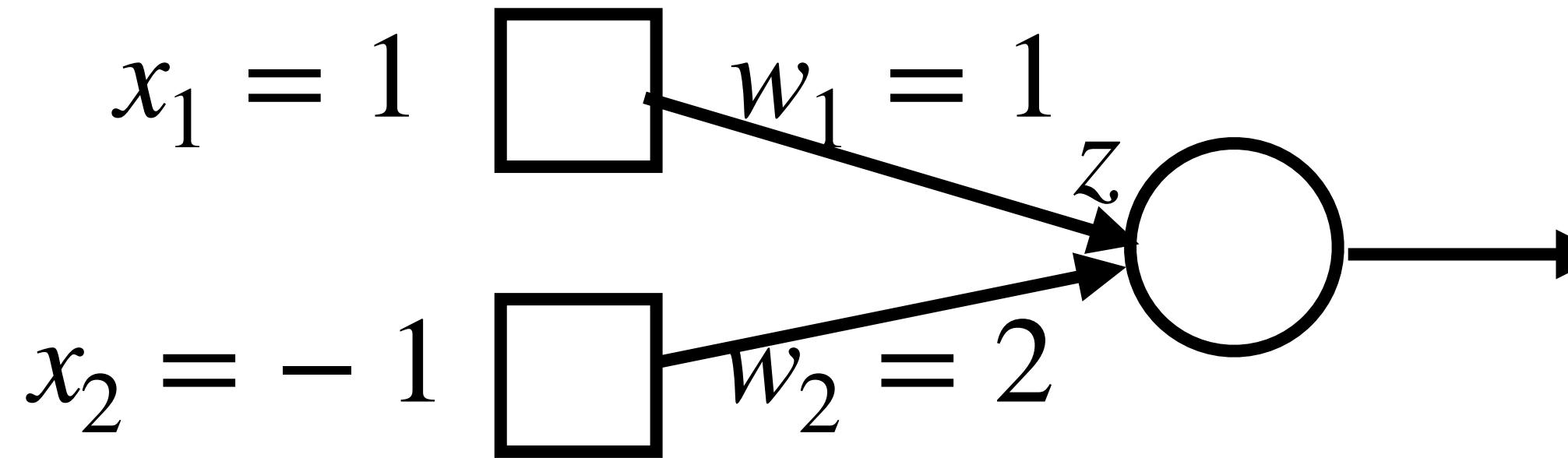
$$z = -1, \hat{y} = \sigma(-1), \ell(\mathbf{x}, y) = -\log \sigma(-1)$$

- Backward:

Example: Backpropagation

$$y = 1$$

$$x_1 = 1$$



sigmoid activation, binary cross-entropy loss

$$\hat{y} = \sigma(w_1x_1 + w_2x_2)$$

$$\ell(\mathbf{x}, y) = -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$$

$$\hat{y} \longrightarrow \ell(\mathbf{x}, y)$$

- Forward:

$$z = -1, \hat{y} = \sigma(-1), \ell(\mathbf{x}, y) = -\log \sigma(-1)$$

- Backward:

$$\frac{\partial \ell}{\partial \hat{y}} = \frac{\partial}{\partial \hat{y}} (-y \log \hat{y} - (1 - y) \log(1 - \hat{y}))$$

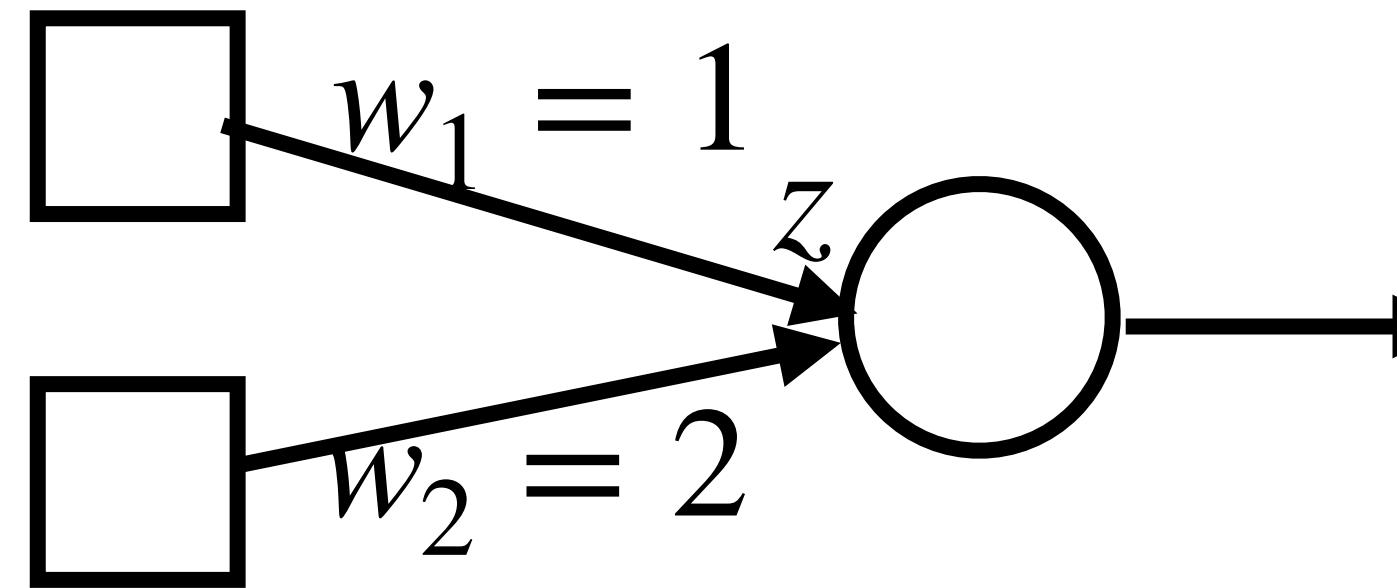
$$= \frac{-y}{\hat{y}} + \frac{1 - y}{1 - \hat{y}} = \frac{\hat{y} - y}{\hat{y}(1 - \hat{y})} = \frac{\sigma(-1) - 1}{\sigma(-1)(1 - \sigma(-1))}$$

Example: Backpropagation

$$y = 1$$

$$x_1 = 1$$

$$x_2 = -1$$



sigmoid activation, binary cross-entropy loss

$$\hat{y} = \sigma(w_1x_1 + w_2x_2)$$

$$\ell(\mathbf{x}, y) = -y \log \hat{y} - (1-y) \log(1-\hat{y})$$

$$\hat{y} \longrightarrow \ell(\mathbf{x}, y)$$

- Forward:

$$z = -1, \hat{y} = \sigma(-1), \ell(\mathbf{x}, y) = -\log \sigma(-1)$$

- Backward:

$$\frac{\partial \ell}{\partial \hat{y}} = \frac{\partial}{\partial \hat{y}} (-y \log \hat{y} - (1-y) \log(1-\hat{y}))$$

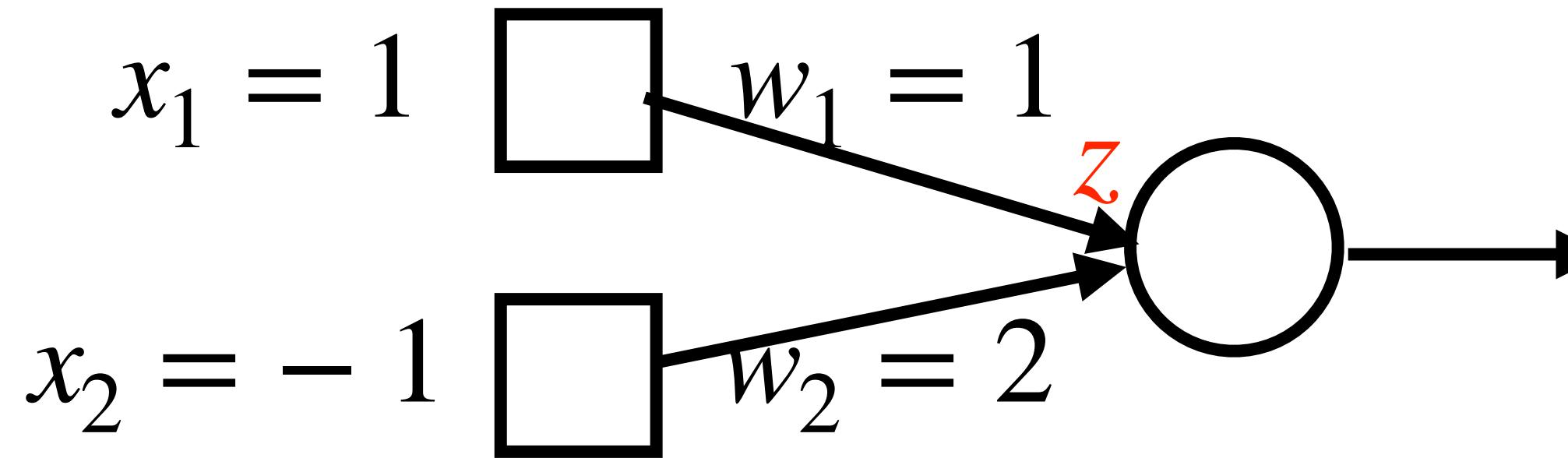
$$= \frac{-y}{\hat{y}} + \frac{1-y}{1-\hat{y}} = \frac{\hat{y}-y}{\hat{y}(1-\hat{y})} = \frac{\sigma(-1)-1}{\sigma(-1)(1-\sigma(-1))}$$

Partial derivative: view all the other variables as constants, and compute the gradient

Example: Backpropagation

$$y = 1$$

$$x_1 = 1$$



sigmoid activation, binary cross-entropy loss

$$\hat{y} = \sigma(w_1x_1 + w_2x_2)$$

$$\ell(\mathbf{x}, y) = -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$$

$$\hat{y} \longrightarrow \ell(\mathbf{x}, y)$$

- Forward:

$$z = -1, \hat{y} = \sigma(-1), \ell(\mathbf{x}, y) = -\log \sigma(-1)$$

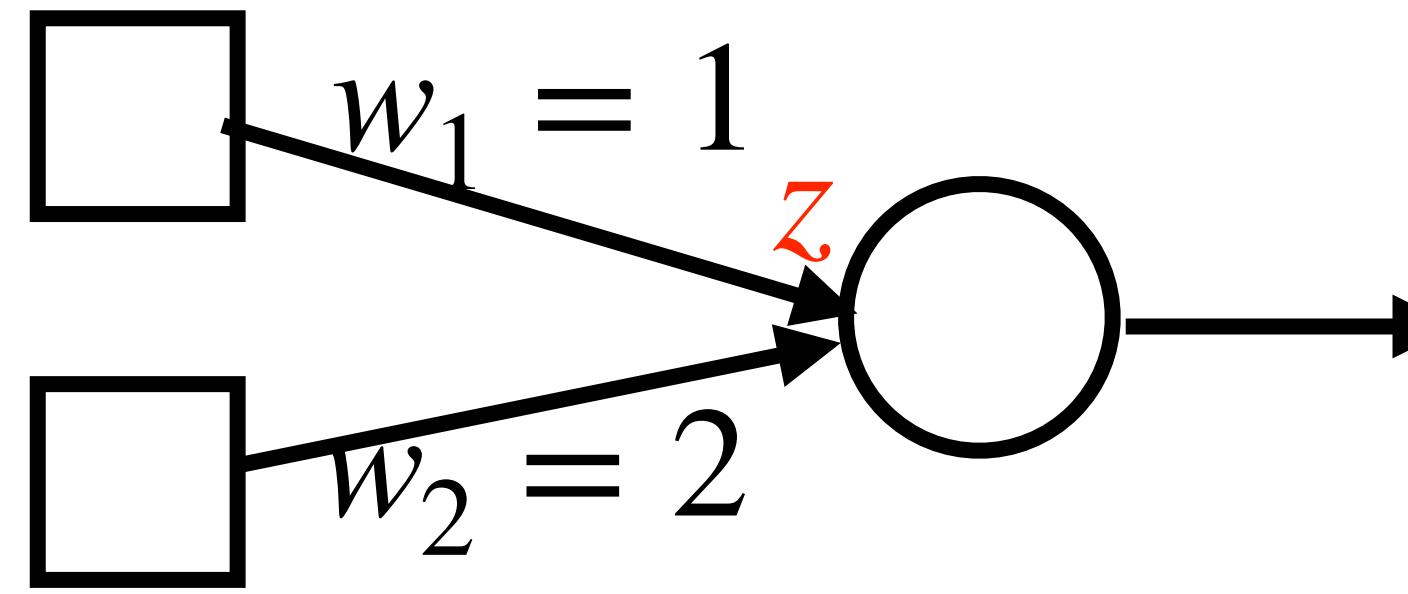
- Backward:
$$\frac{\partial \ell}{\partial \hat{y}} = \frac{\sigma(-1) - 1}{\sigma(-1)(1 - \sigma(-1))}$$

Example: Backpropagation

$$y = 1$$

$$x_1 = 1$$

$$x_2 = -1$$



sigmoid activation, binary cross-entropy loss

$$\hat{y} = \sigma(w_1 x_1 + w_2 x_2)$$

$$\ell(\mathbf{x}, y) = -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$$

$$\hat{y} \longrightarrow \ell(\mathbf{x}, y)$$

- Forward:

$$z = -1, \hat{y} = \sigma(-1), \ell(\mathbf{x}, y) = -\log \sigma(-1)$$

- Backward: $\frac{\partial \ell}{\partial \hat{y}} = \frac{\sigma(-1) - 1}{\sigma(-1)(1 - \sigma(-1))}$

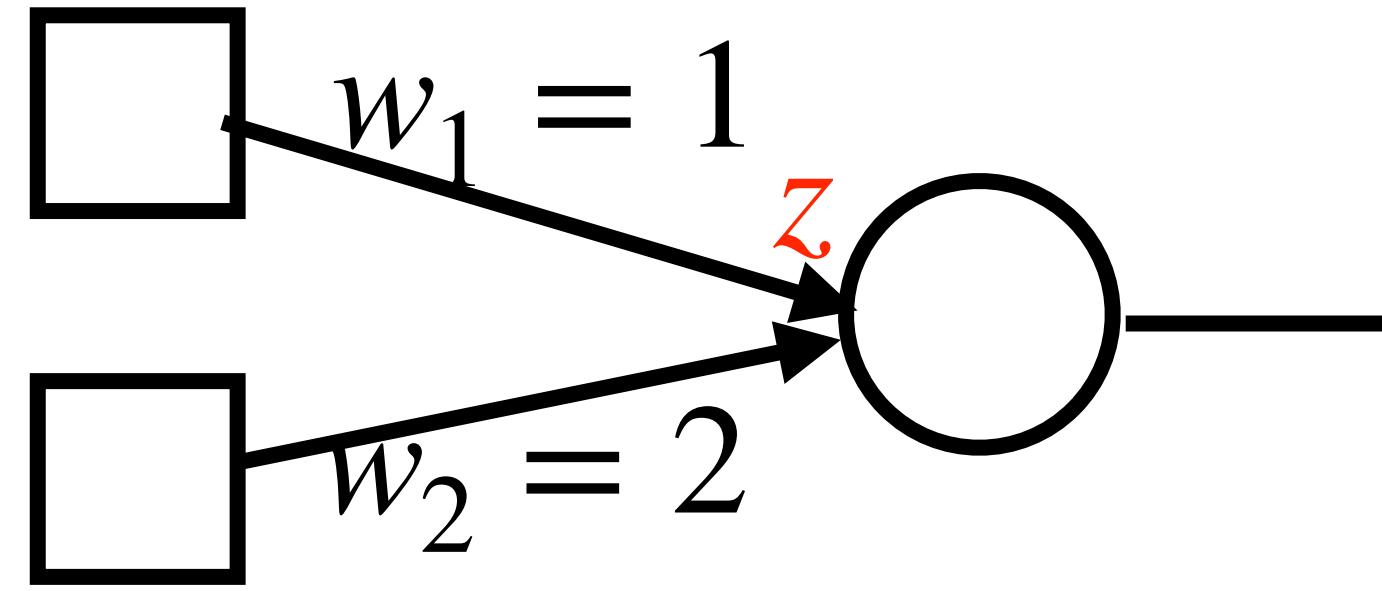
$$\frac{\partial \ell}{\partial z} = \frac{\partial \ell}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z}$$

Example: Backpropagation

$$y = 1$$

$$x_1 = 1$$

$$x_2 = -1$$



sigmoid activation, binary cross-entropy loss

$$\hat{y} = \sigma(w_1x_1 + w_2x_2)$$

$$\ell(\mathbf{x}, y) = -y \log \hat{y} - (1-y) \log(1-\hat{y})$$

- Forward:

$$z = -1, \hat{y} = \sigma(-1), \ell(\mathbf{x}, y) = -\log \sigma(-1)$$

- Backward:

$$\frac{\partial \ell}{\partial z} = \frac{\partial \ell}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z}$$

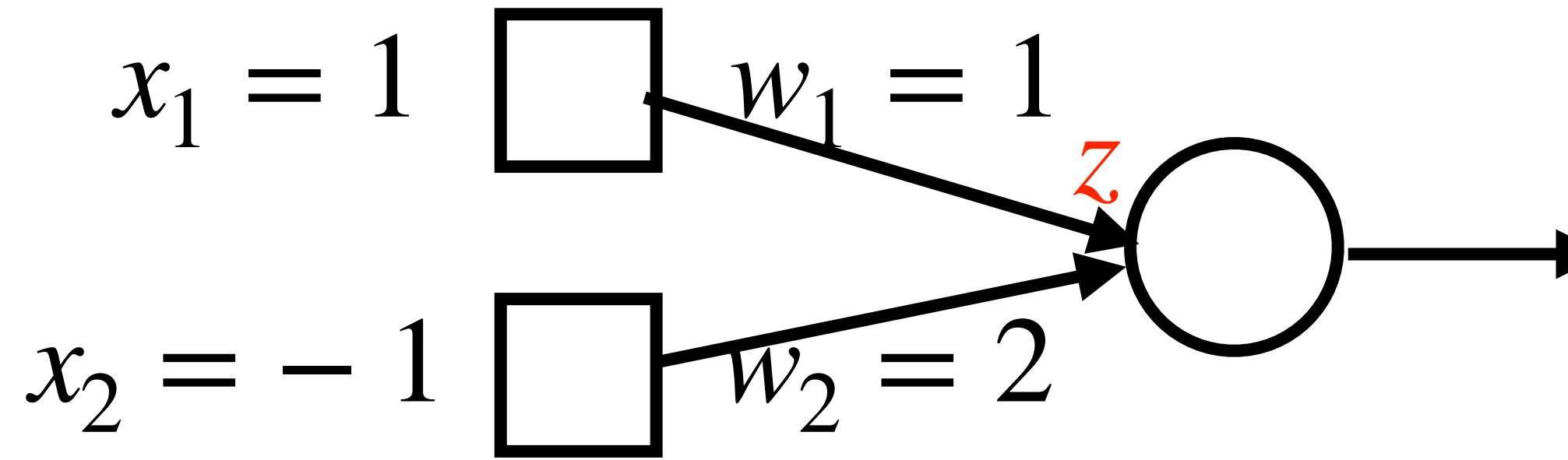
$$\frac{\partial \ell}{\partial \hat{y}} = \frac{\sigma(-1) - 1}{\sigma(-1)(1 - \sigma(-1))}$$

$$\frac{\partial \hat{y}}{\partial z} = \frac{\partial}{\partial z} \sigma(z) = \sigma(z)(1 - \sigma(z)) = \hat{y}(1 - \hat{y}) = \sigma(-1)(1 - \sigma(-1))$$

Example: Backpropagation

$$y = 1$$

$$x_1 = 1$$



sigmoid activation, binary cross-entropy loss

$$\hat{y} = \sigma(w_1x_1 + w_2x_2)$$

$$\ell(\mathbf{x}, y) = -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$$

$$\hat{y} \longrightarrow \ell(\mathbf{x}, y)$$

- Forward:

$$z = -1, \hat{y} = \sigma(-1), \ell(\mathbf{x}, y) = -\log \sigma(-1)$$

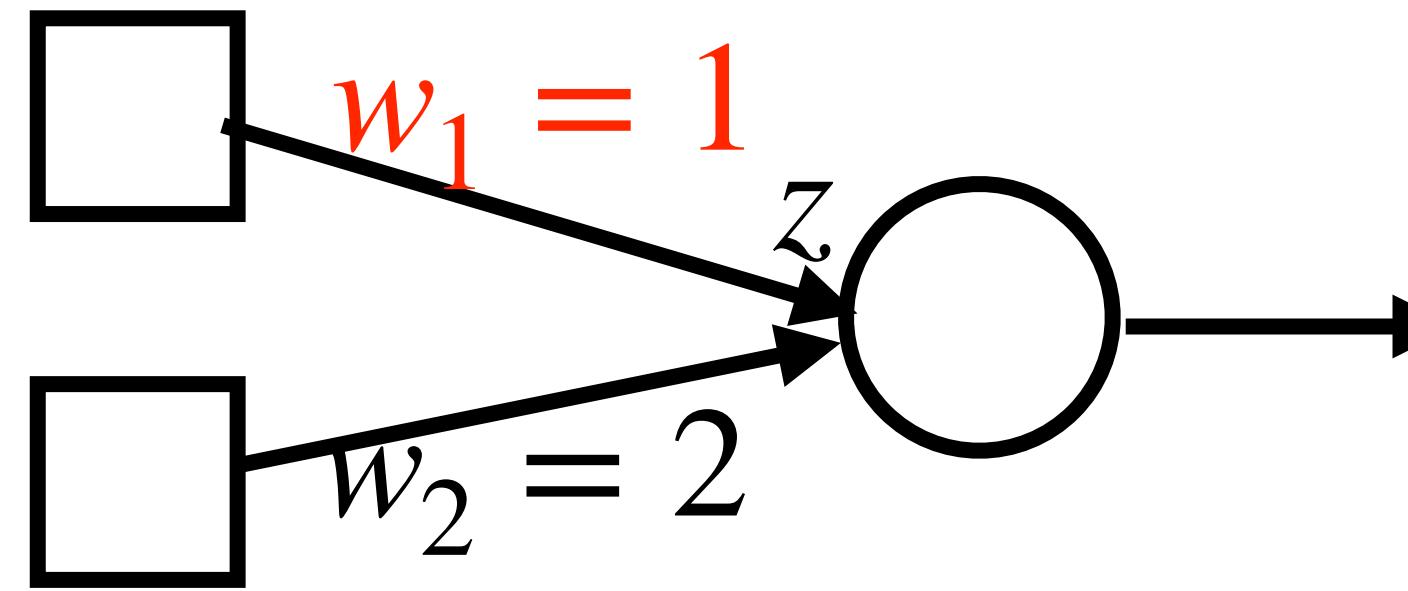
- Backward: $\frac{\partial \ell}{\partial z} = \frac{\partial \ell}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z} = \sigma(-1) - 1$

Example: Backpropagation

$$y = 1$$

$$x_1 = 1$$

$$x_2 = -1$$



$$\hat{y} = \sigma(w_1 x_1 + w_2 x_2)$$

$$\ell(\mathbf{x}, y) = -y \log \hat{y} - (1-y) \log(1-\hat{y})$$

$$\hat{y} \longrightarrow \ell(\mathbf{x}, y)$$

- Forward:

$$z = -1, \hat{y} = \sigma(-1), \ell(\mathbf{x}, y) = -\log \sigma(-1)$$

- Backward: $\frac{\partial \ell}{\partial z} = \frac{\partial \ell}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z} = \sigma(-1) - 1$

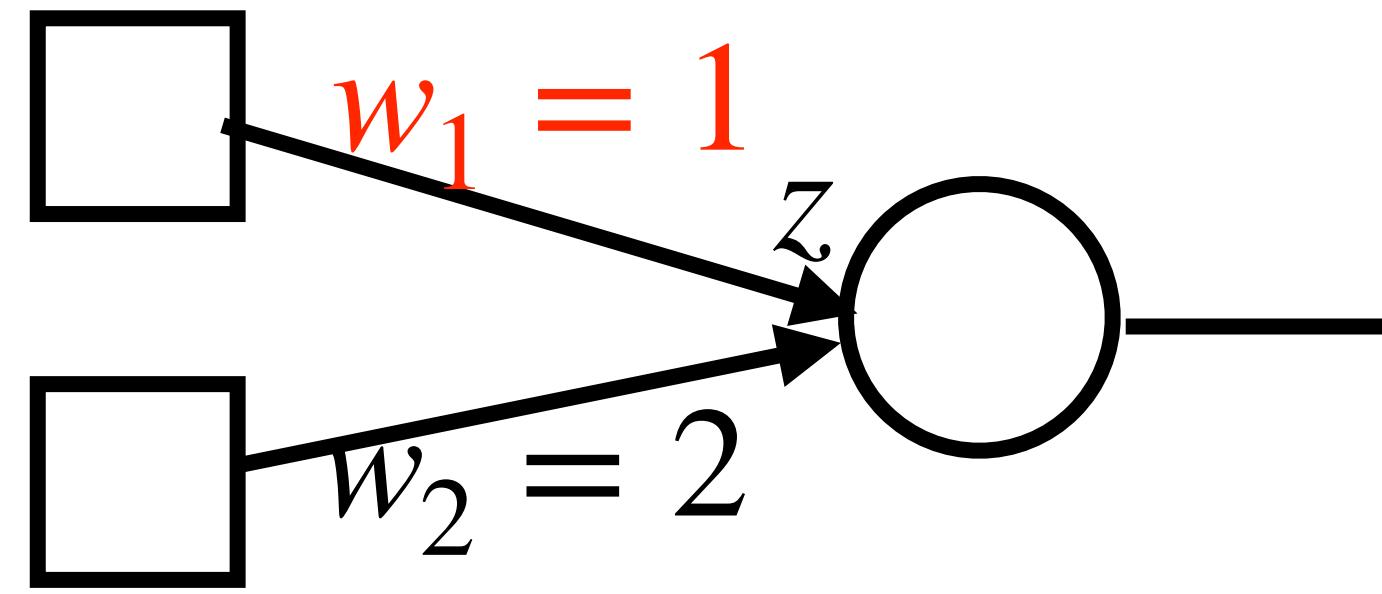
$$\frac{\partial \ell}{\partial w_1} = \frac{\partial \ell}{\partial z} \frac{\partial z}{\partial w_1}$$

Example: Backpropagation

$$y = 1$$

$$x_1 = 1$$

$$x_2 = -1$$



sigmoid activation, binary cross-entropy loss

$$\hat{y} = \sigma(w_1x_1 + w_2x_2)$$

$$\ell(\mathbf{x}, y) = -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$$

$$\hat{y} \longrightarrow \ell(\mathbf{x}, y)$$

- Forward:

$$z = -1, \hat{y} = \sigma(-1), \ell(\mathbf{x}, y) = -\log \sigma(-1)$$

- Backward:

$$\frac{\partial \ell}{\partial z} = \frac{\partial \ell}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial z} = \sigma(-1) - 1$$

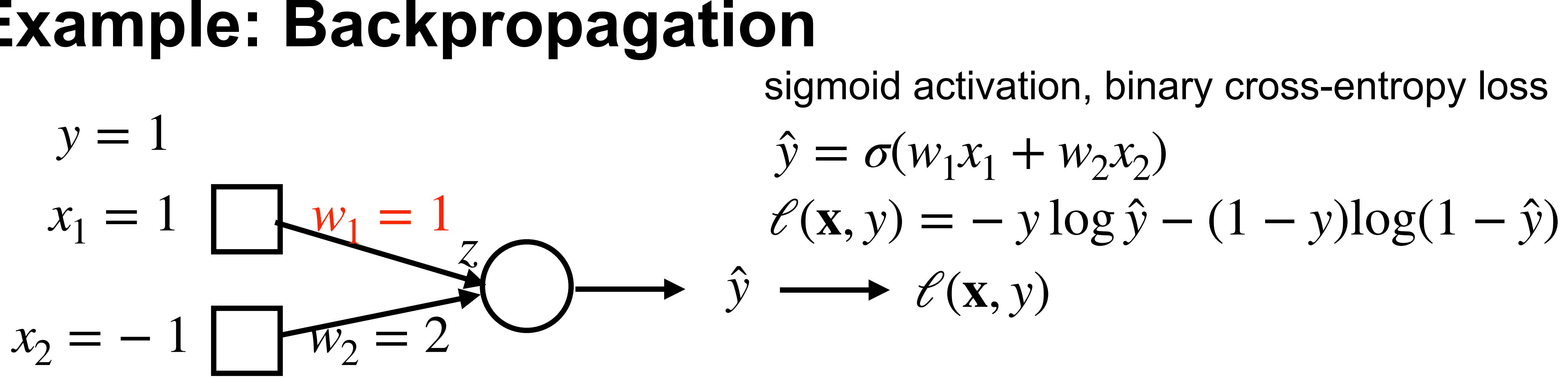
$$\frac{\partial \ell}{\partial w_1} = \frac{\partial \ell}{\partial z} \frac{\partial z}{\partial w_1}$$

$$\frac{\partial z}{\partial w_1} = \frac{\partial}{\partial w_1}(w_1x_1 + w_2x_2) = x_1 = 1$$

Example: Backpropagation

$$y = 1$$

$$x_1 = 1$$



- Forward:

$$z = -1, \hat{y} = \sigma(-1), \ell(\mathbf{x}, y) = -\log \sigma(-1)$$

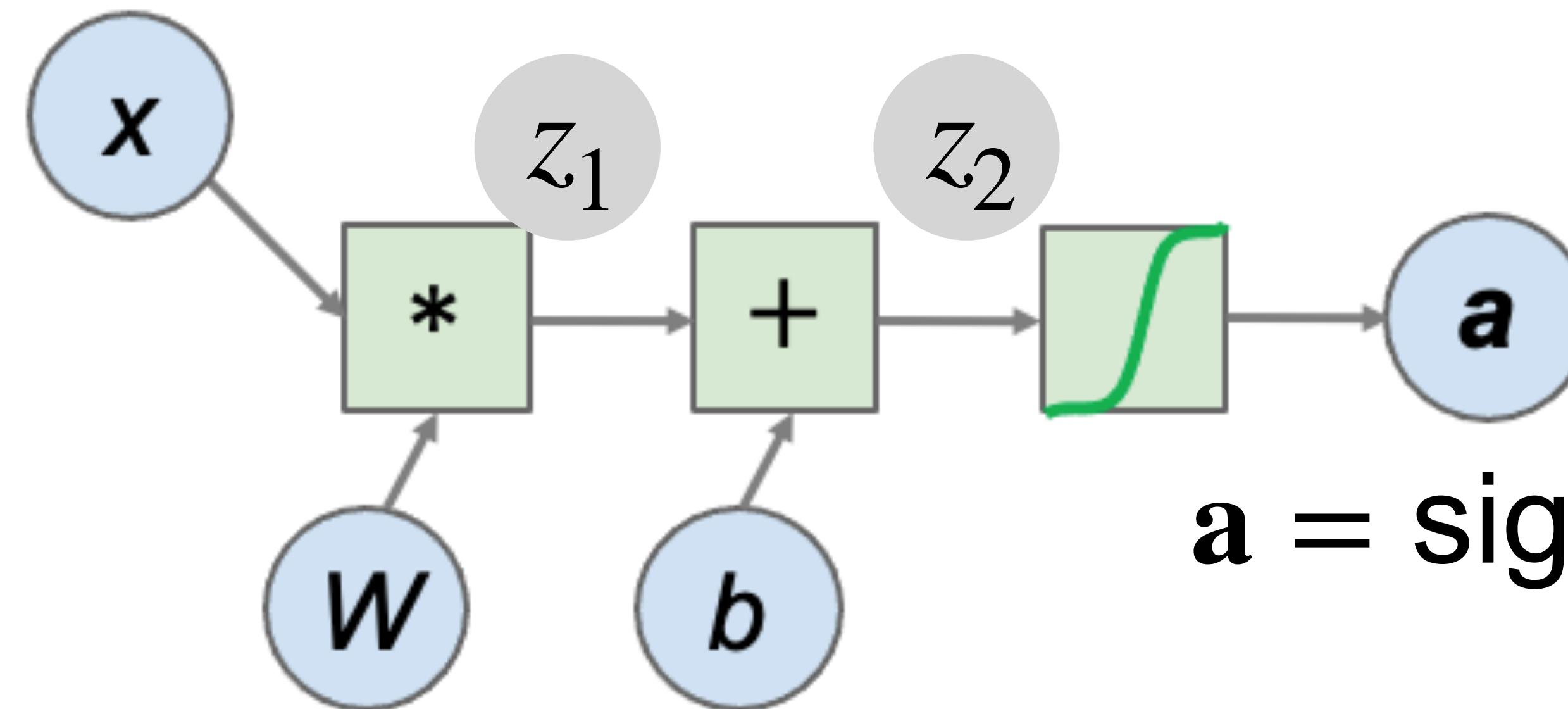
- Backward:

$$\frac{\partial \ell}{\partial w_1} = \frac{\partial \ell}{\partial z} \frac{\partial z}{\partial w_1} = (\sigma(-1) - 1) \times 1 = \sigma(-1) - 1$$

Calculate Gradient: Backpropagation with Chain Rule

- Define a loss function L
- Gradient to a variable =
gradient on the top \times gradient from the current operation

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



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

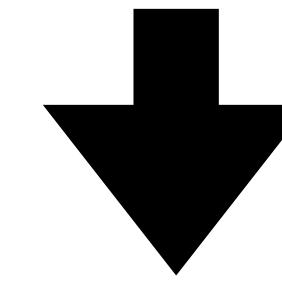
Convolutional Neural Networks



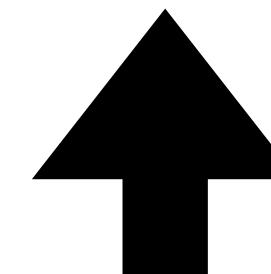
2-D Convolution Layer with Stride and Padding

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

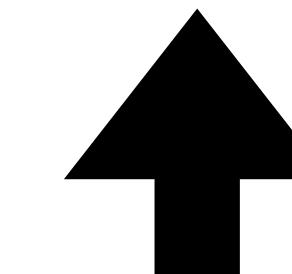
Kernel/filter size



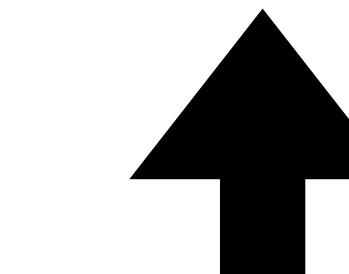
$$\lfloor (n_h - k_h + p_h + s_h) / s_h \rfloor \times \lfloor (n_w - k_w + p_w + s_w) / s_w \rfloor$$



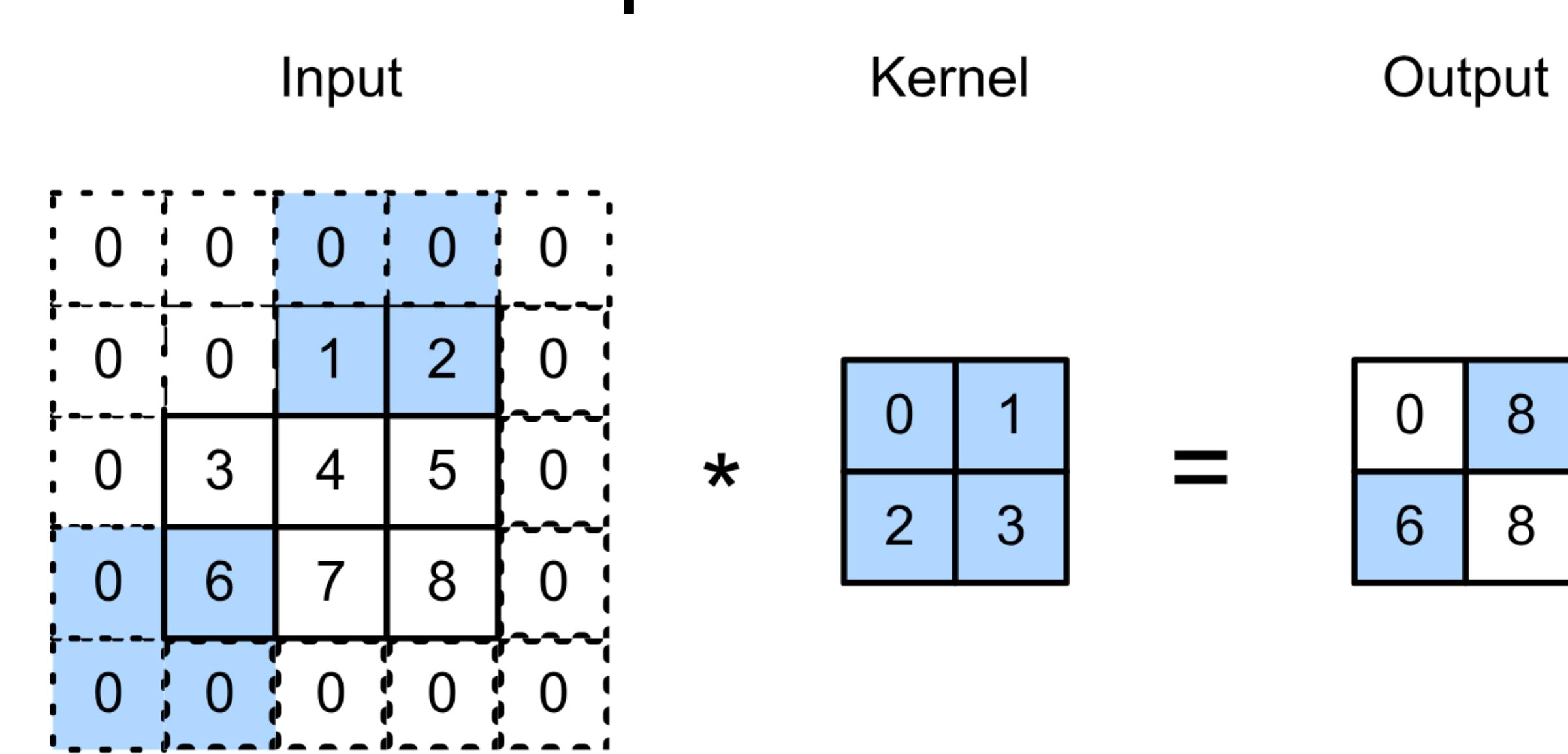
Input size



Pad

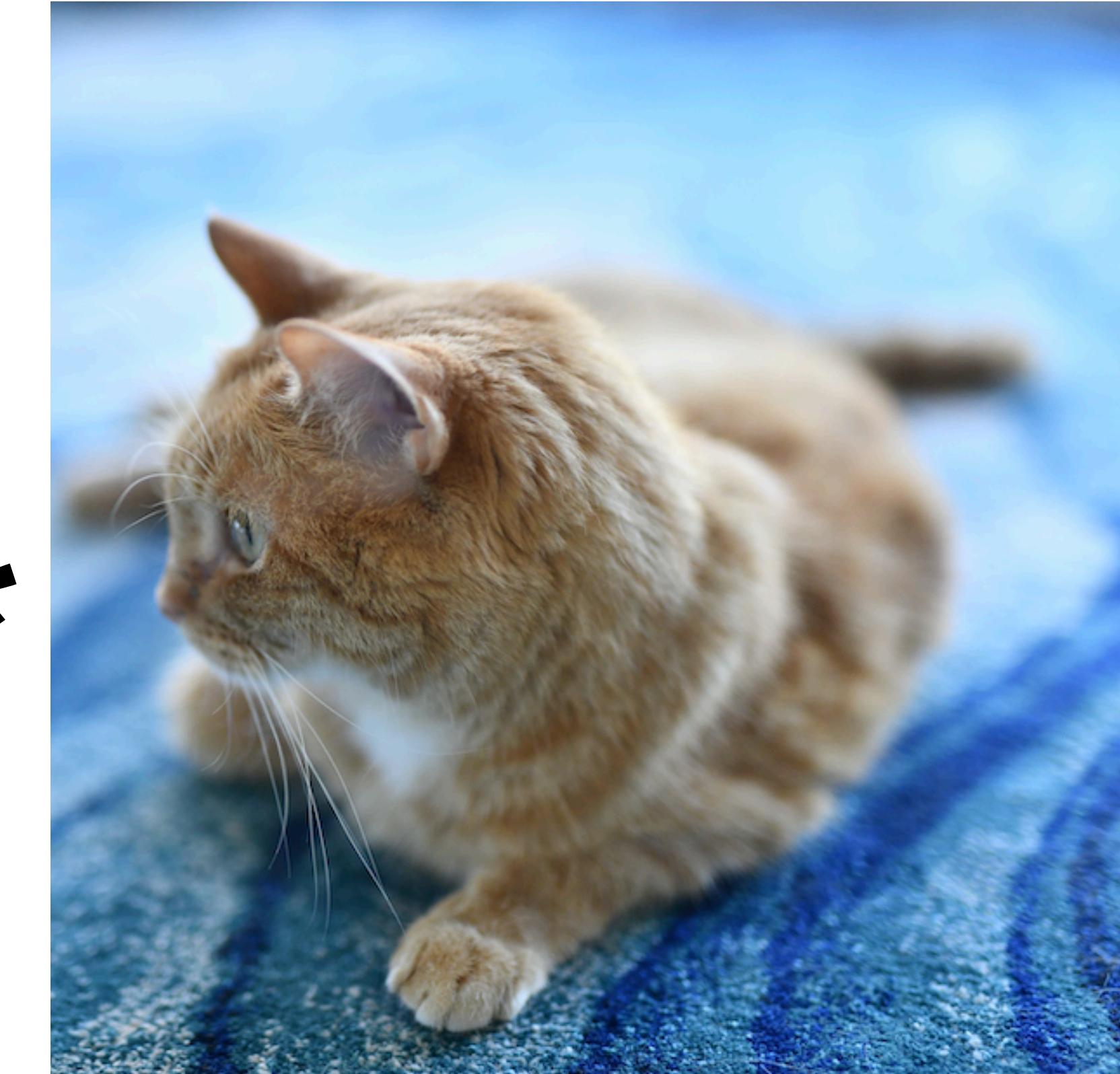
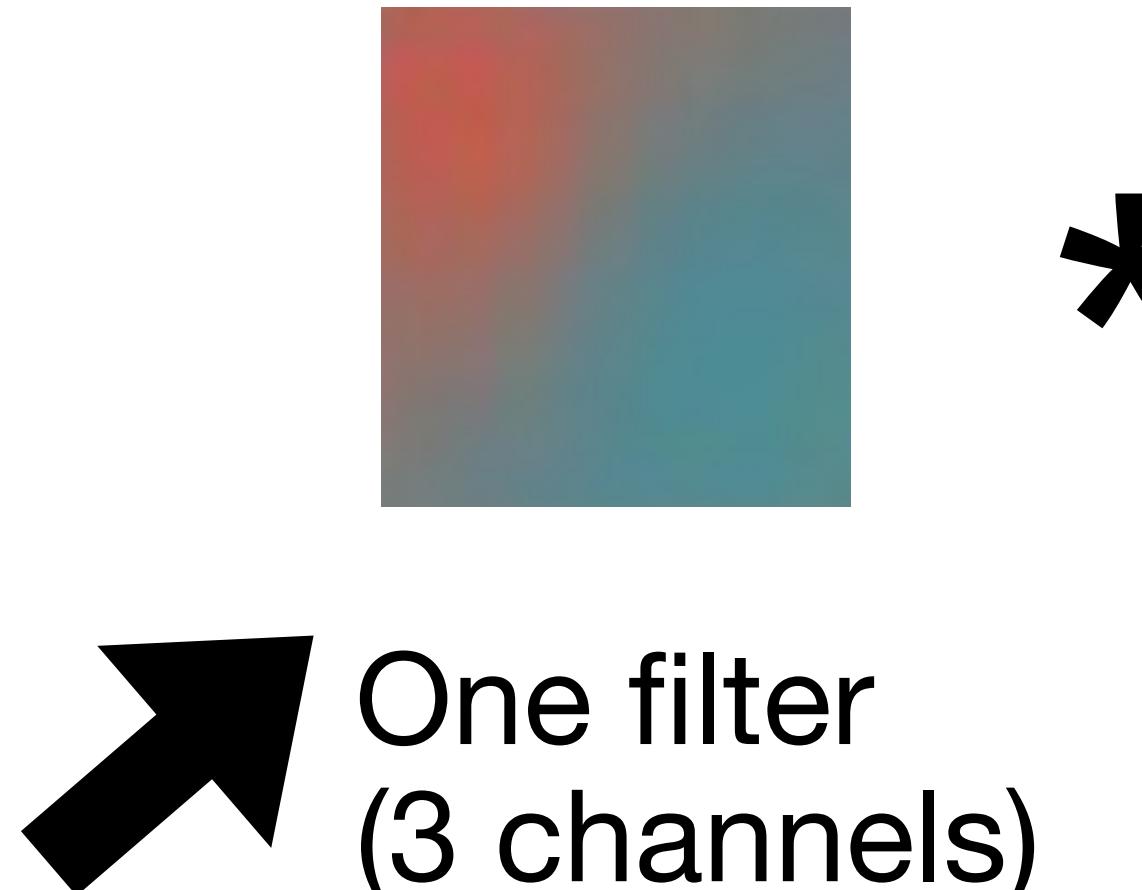


Stride



Multiple Input Channels

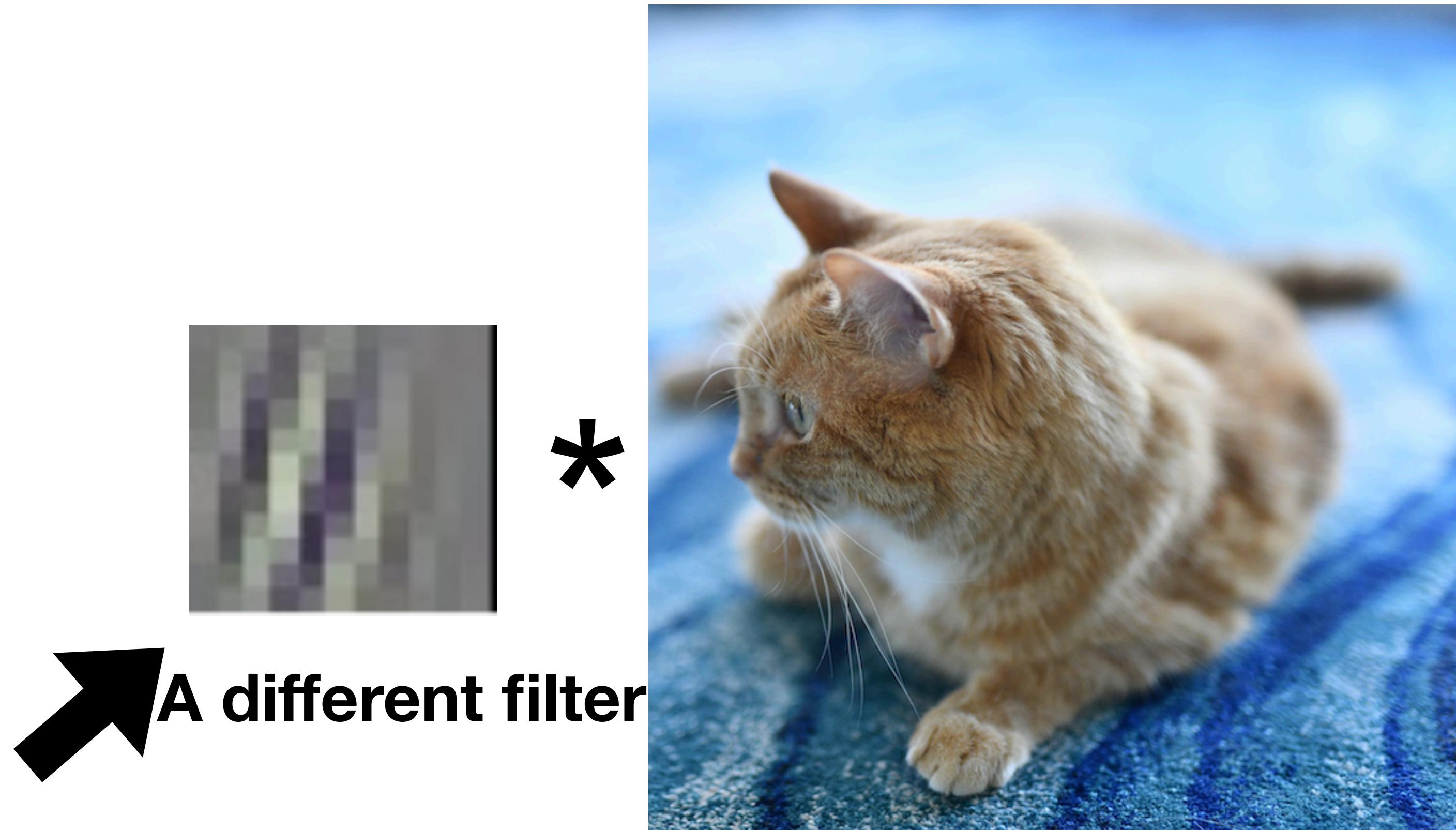
- Input and kernel can be 3D, e.g., an RGB image have 3 channels
- Also call each 3D kernel a “**filter**”, which produce only **one** output channel (due to summation over channels)



RGB (3 input channels)

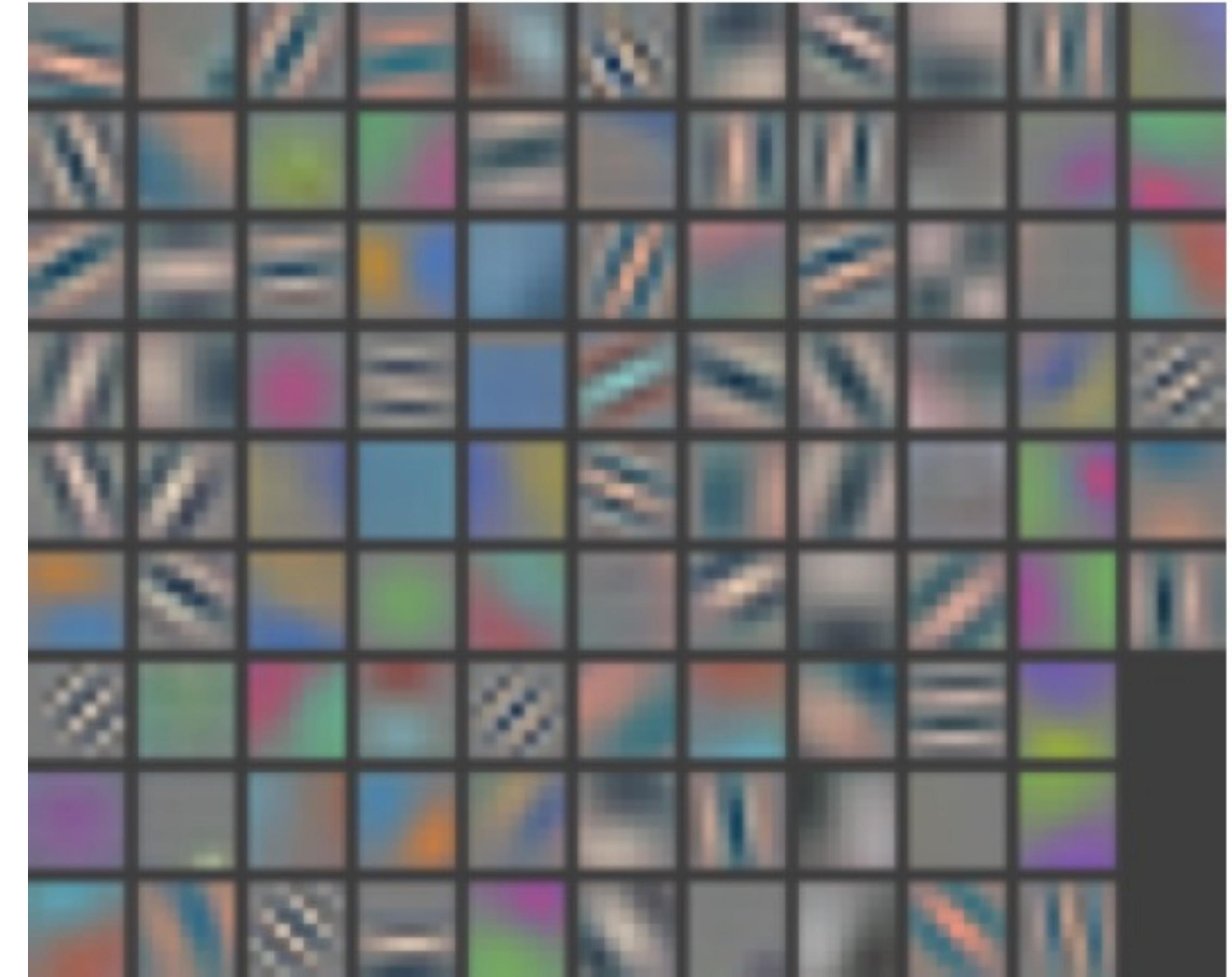
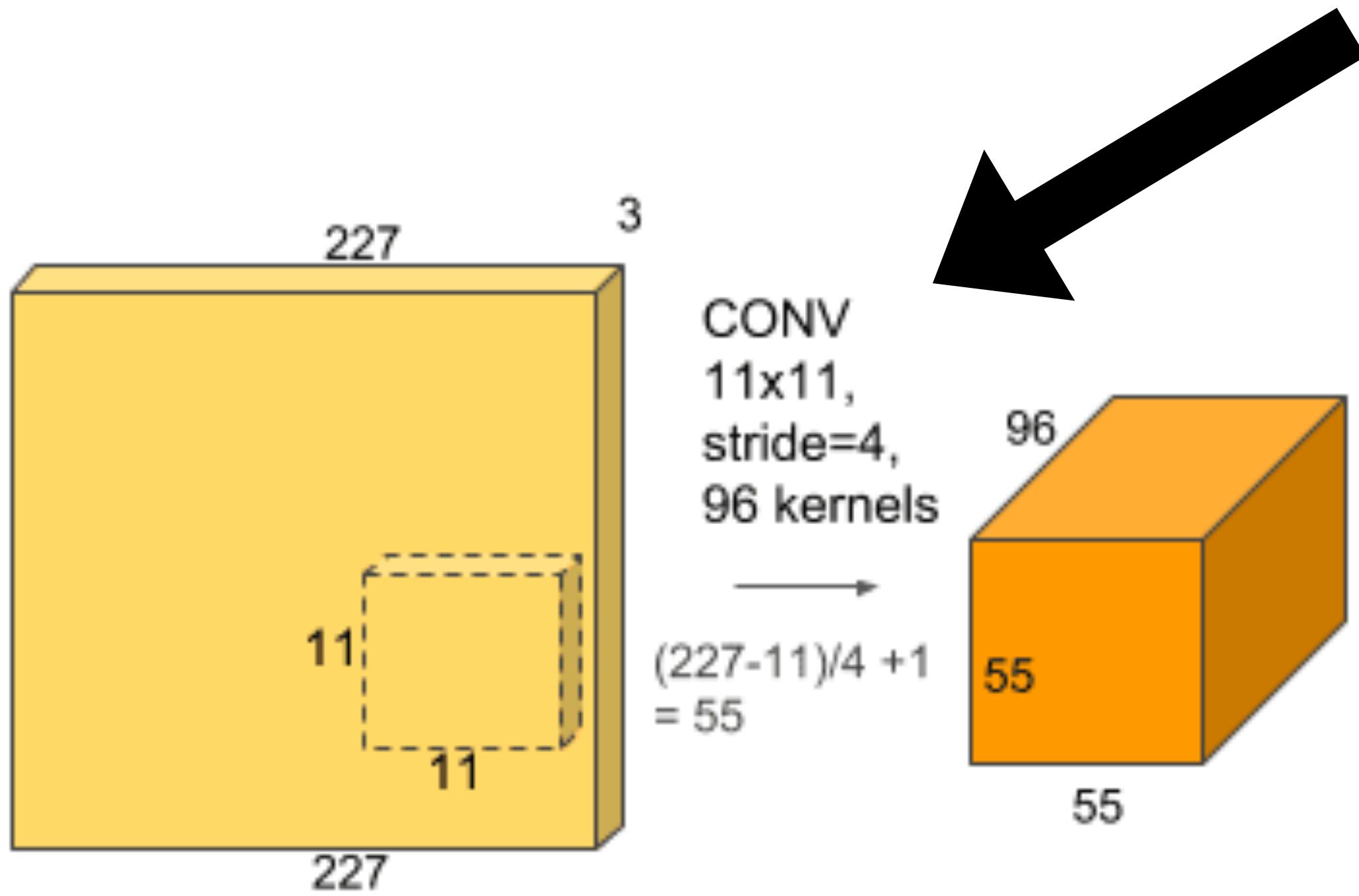
Multiple Filters Lead to Multiple Output Channels

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



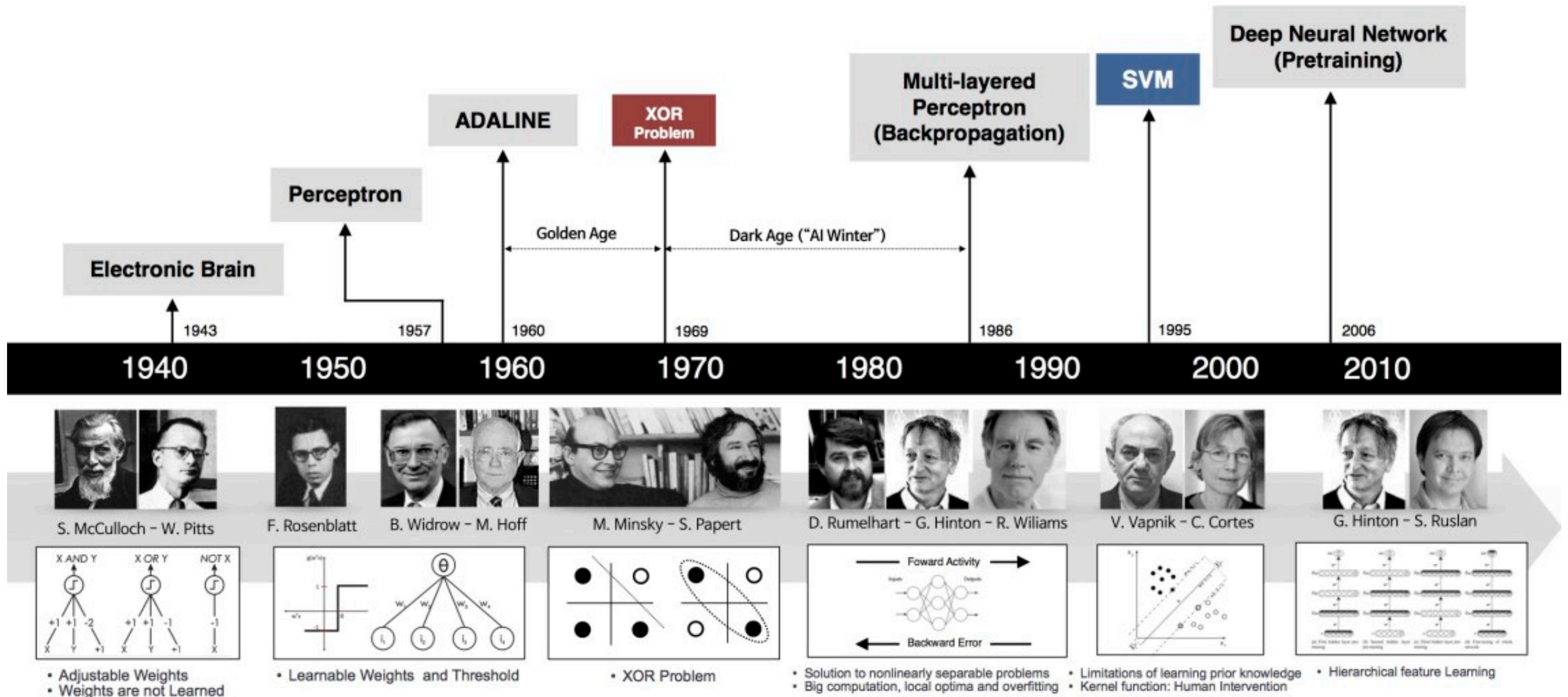
Conv1 Filters in AlexNet

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

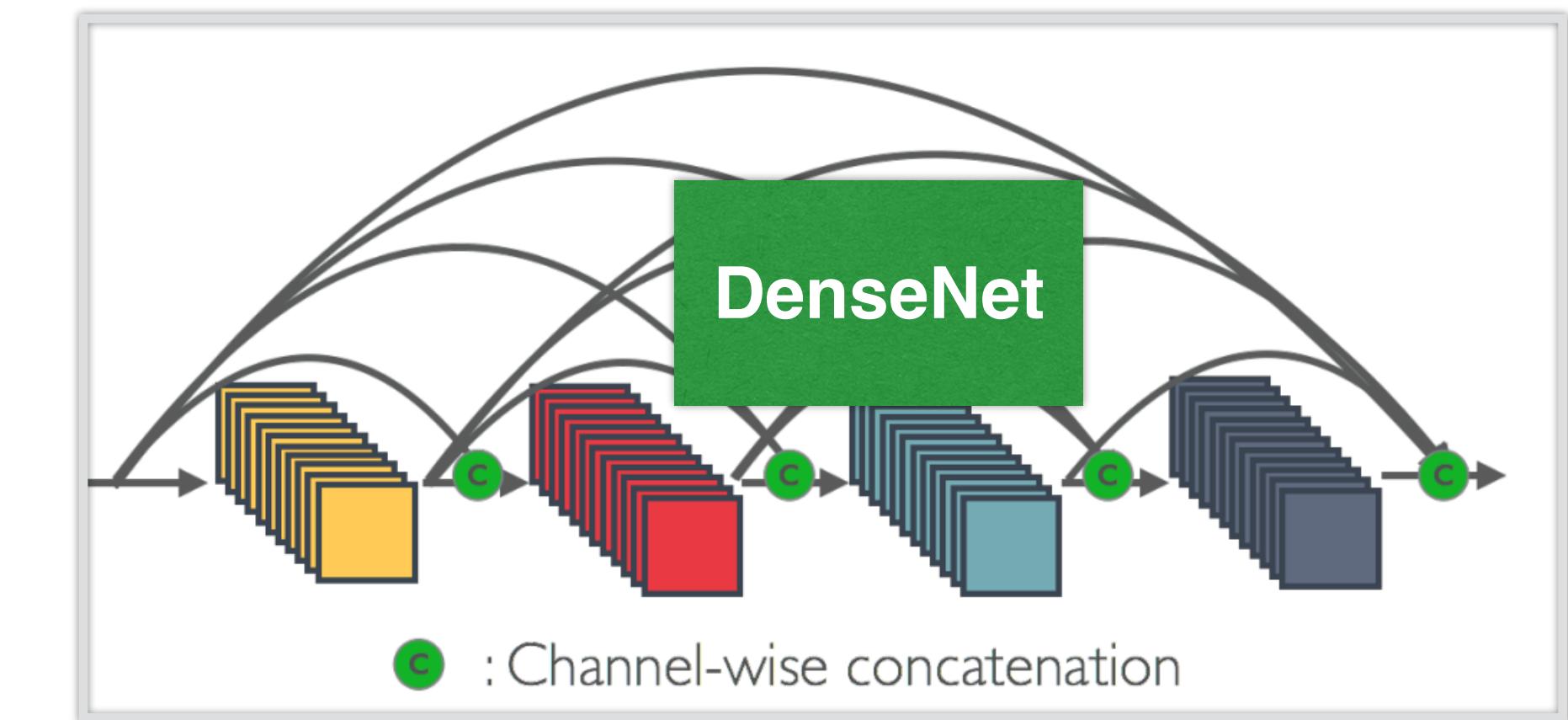
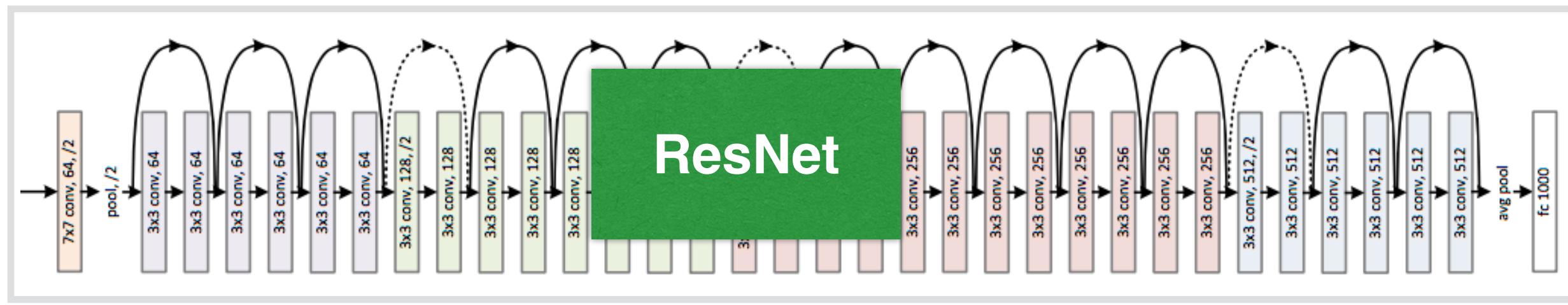
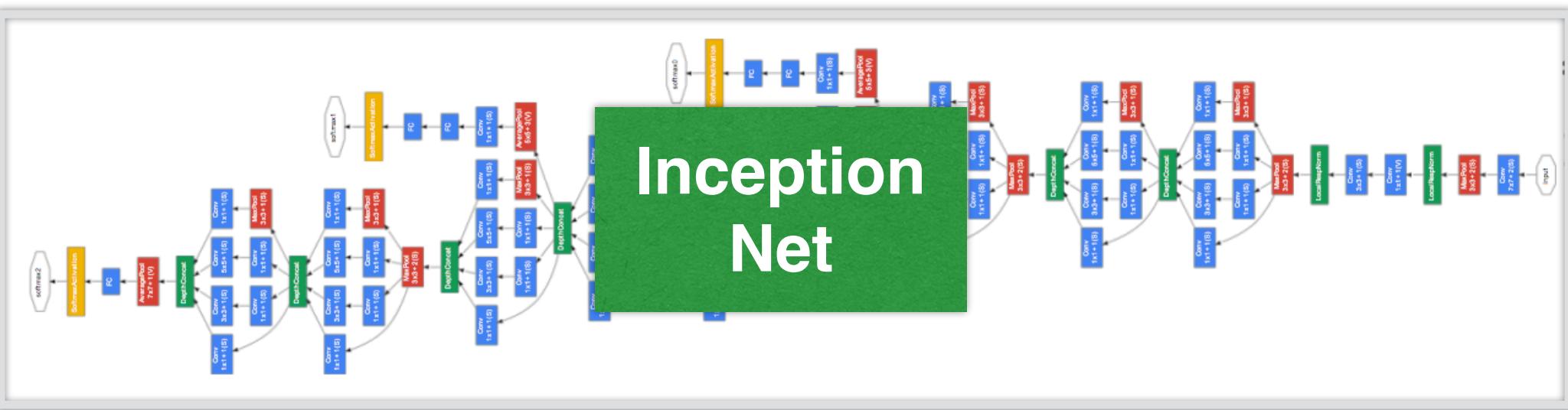
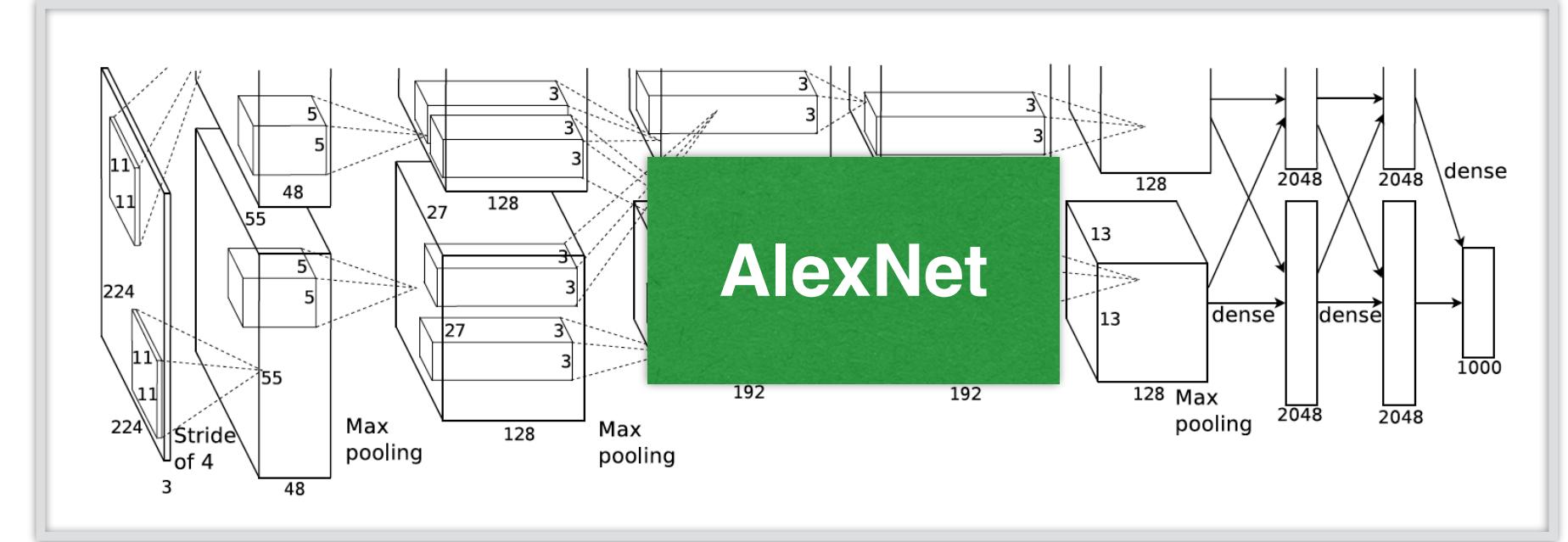
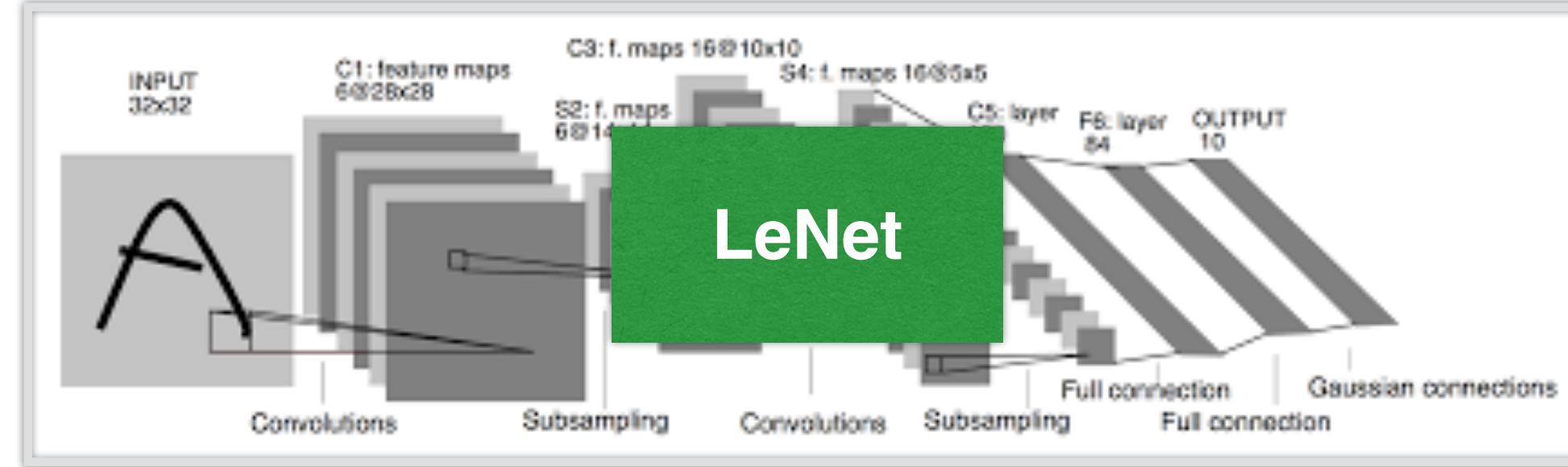


Figures from Visualizing and Understanding Convolutional Networks
by M. Zeiler and R. Fergus

Brief history of neural networks



Evolution of modern deep neural net architectures



What we've learned today...

- Modeling a single neuron
 - 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>