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10th March 2020



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Introduction to deep learning

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“When you’re **fundraising**, it’s AI

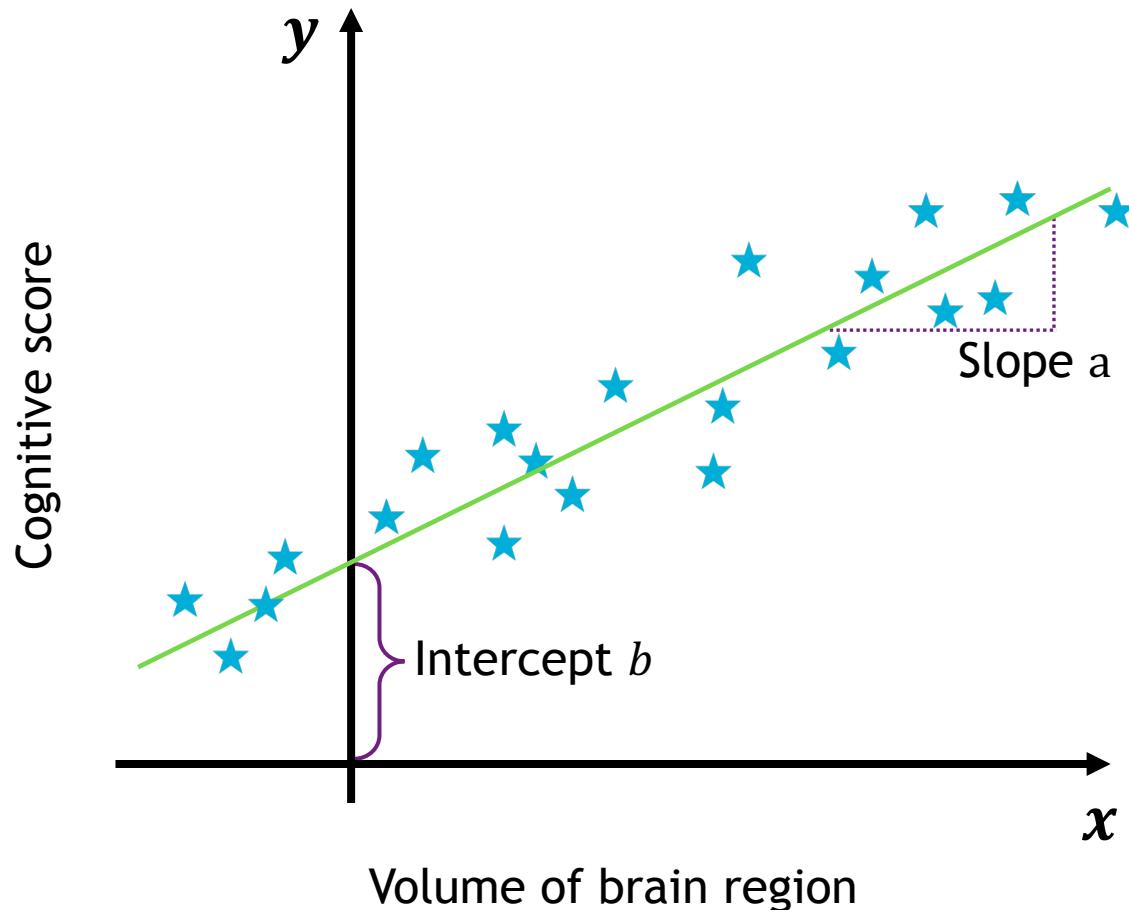
When you’re **hiring**, it’s ML

When you’re **implementing**, it’s linear regression”

— Baron Schwartz

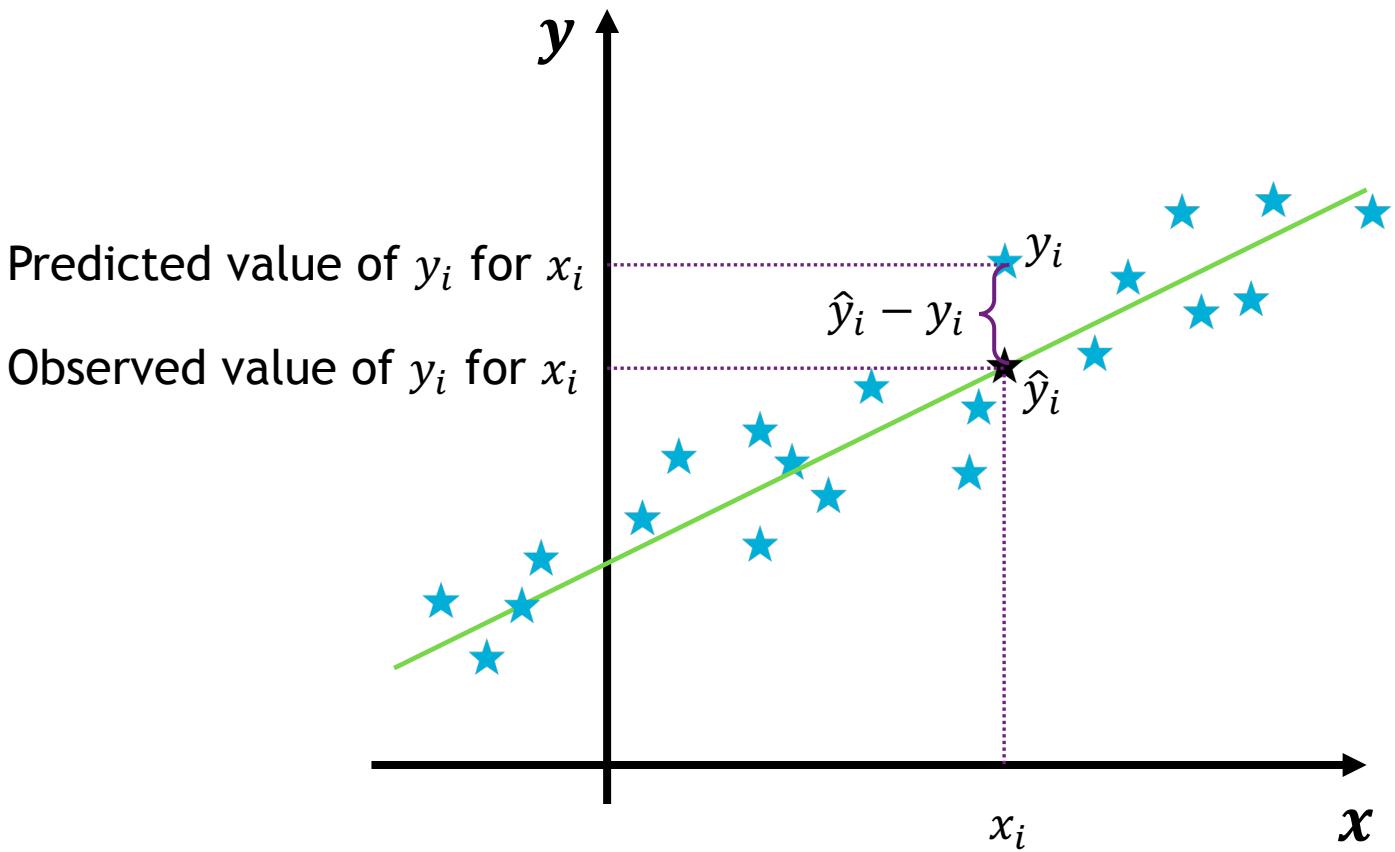
The basics

What is linear regression?



$$y = f(x) = ax + b$$

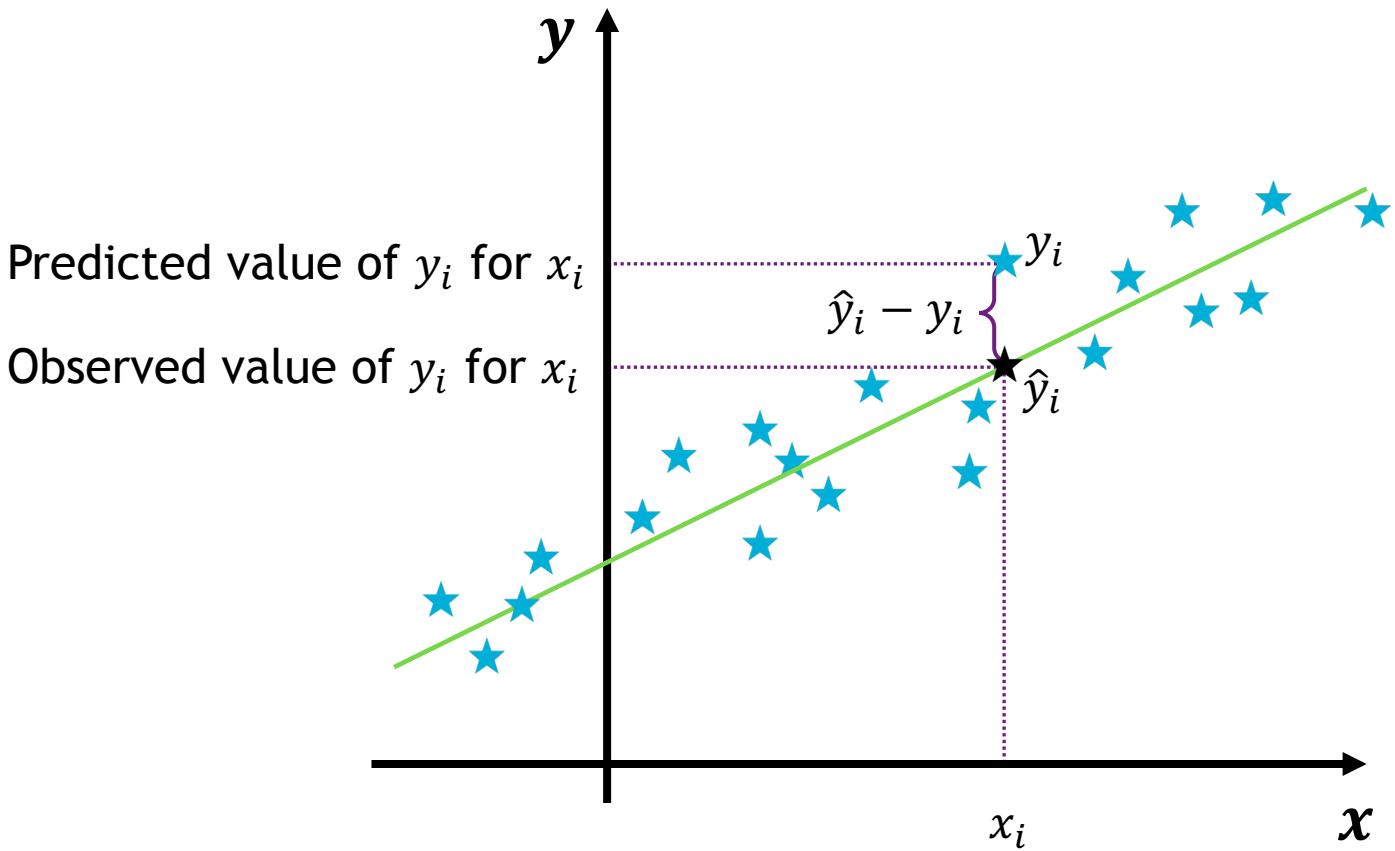
Cost function



Mean squared error:

$$J = \frac{1}{n} \sum_{i=1}^n (\hat{y}_i - y_i)^2$$

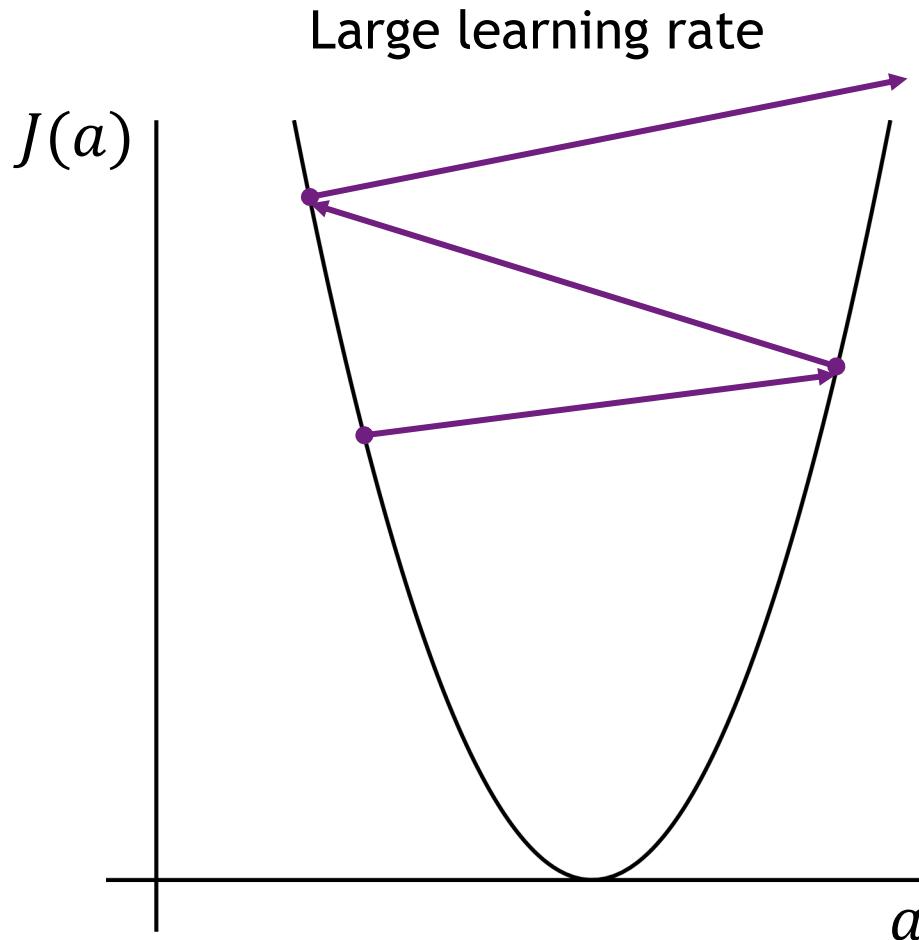
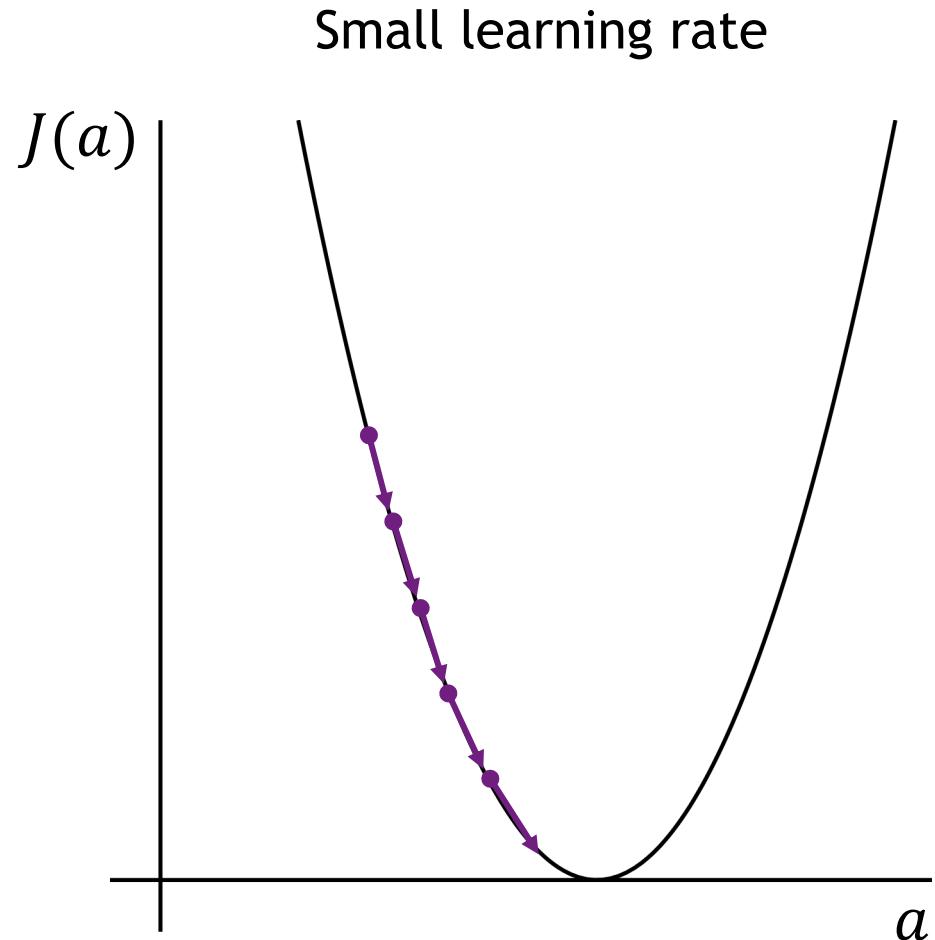
Learning



Find the model with the minimal error:

$$\hat{f} = \arg \min_{f \in \mathcal{F}} J(f)$$

Gradient descent



Gradient descent

Cost function:

$$J = \frac{1}{n} \sum_{i=1}^n (\hat{y}_i - y_i)^2 = \frac{1}{n} \sum_{i=1}^n (ax_i + b - y_i)^2$$

Partial derivate:

$$\frac{\partial J}{\partial a} = \frac{2}{n} \sum_{i=1}^n (ax_i + b - y_i) \cdot x_i = \frac{2}{n} \sum_{i=1}^n (\hat{y}_i - y_i) \cdot x_i$$

$$\frac{\partial J}{\partial b} = \frac{2}{n} \sum_{i=1}^n (ax_i + b - y_i) = \frac{2}{n} \sum_{i=1}^n (\hat{y}_i - y_i)$$

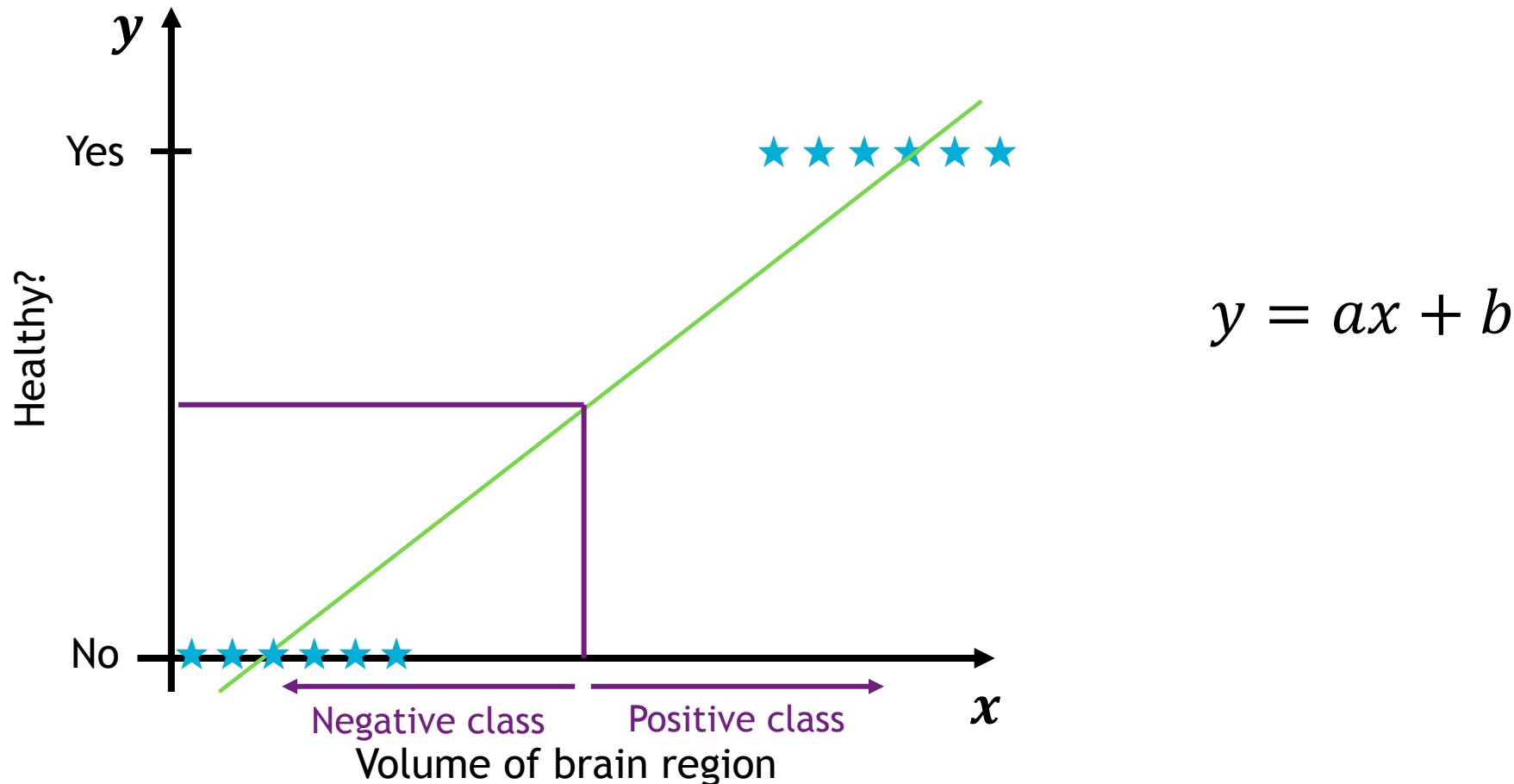
Update of a and b :

$$a \leftarrow a - \eta \frac{\partial J}{\partial a} = a - \eta \frac{2}{n} \sum_{i=1}^n (\hat{y}_i - y_i)$$

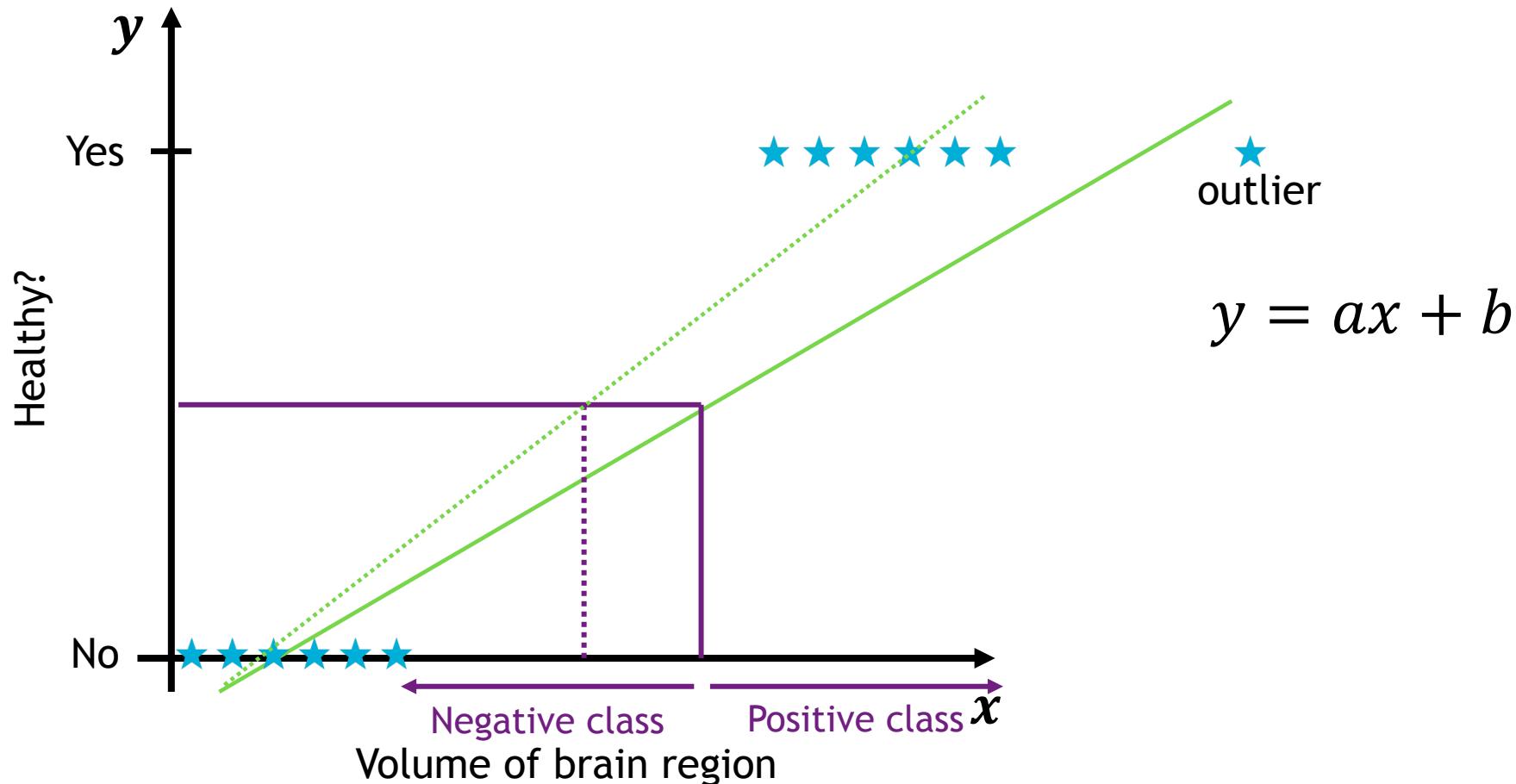
$$b \leftarrow b - \eta \frac{\partial J}{\partial b} = b - \eta \frac{2}{n} \sum_{i=1}^n (\hat{y}_i - y_i) \cdot x_i$$

Logistic regression

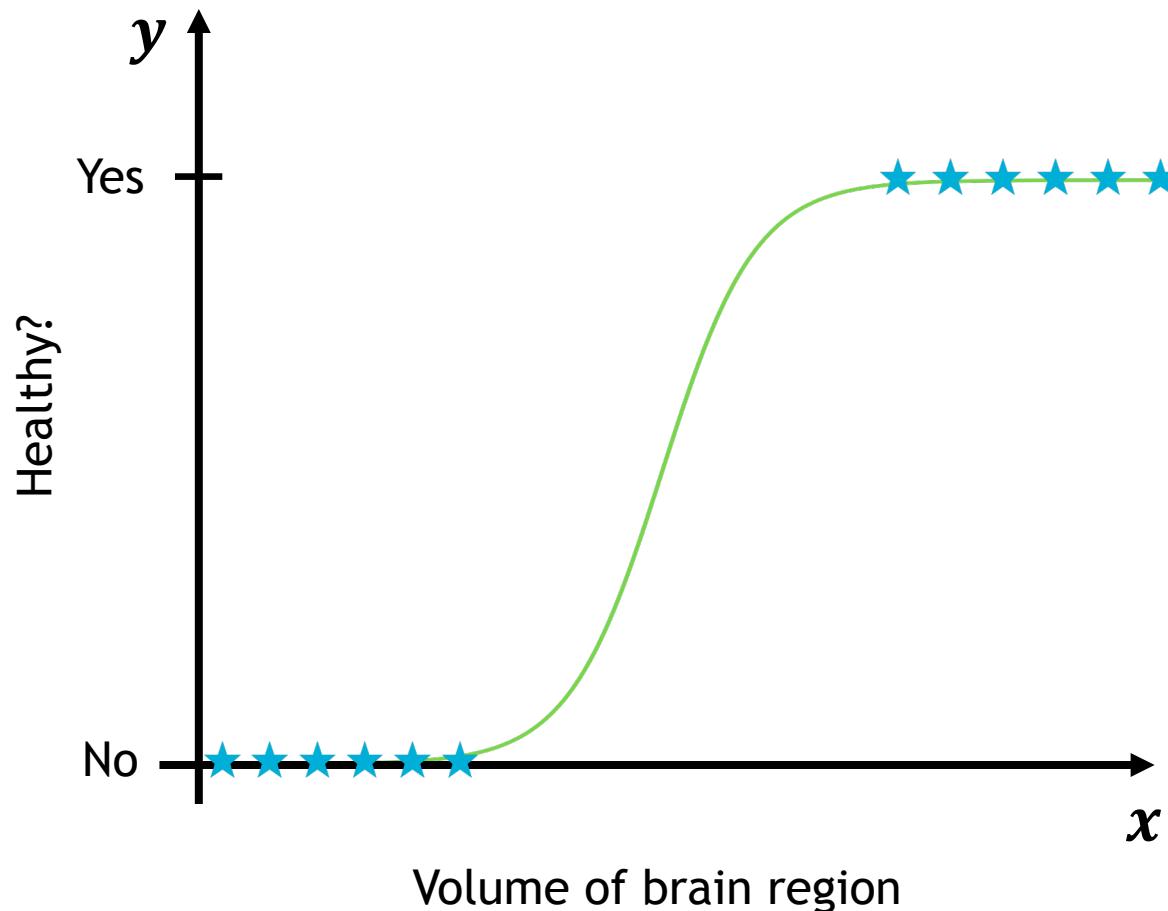
Linear function



Linear function



Sigmoid function



$$y = ax + b$$

$$f = \frac{1}{1 + e^{-y}} = \frac{1}{1 + e^{-(ax+b)}}$$

Multiple input variables

$$z = w_0 + w_1 x_1 + w_2 x_2 + \cdots + w_m x_m = w_0 + \sum_{j=1}^m x_j w_j$$

$$f = \frac{1}{1 + e^{-z}} = \frac{1}{1 + e^{-(w_0 + \sum_{j=1}^m x_j w_j)}}$$

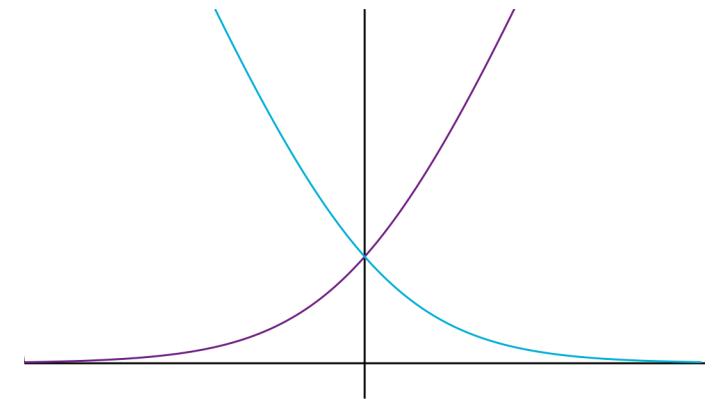
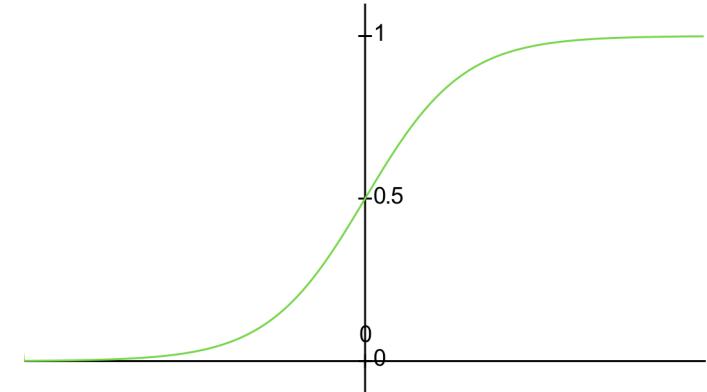
Loss function

- Low if prediction is correct
- High if prediction is wrong

$\begin{cases} \text{if } y = 1, l(f(x), y) \text{ should be low when } f(x) \text{ is high} \\ \text{if } y = 0, l(f(x), y) \text{ should be low when } f(x) \text{ is low} \end{cases}$

$$l(f(x), y) = \begin{cases} -\log(f(x)), & \text{if } y = 1 \\ -\log(1 - f(x)), & \text{if } y = 0 \end{cases}$$

$$l(f(x), y) = -y \log(f(x)) - (1 - y) \log(1 - f(x))$$



Cost function

$$J(f) = \frac{1}{n} \sum_{i=1}^n l(f(\mathbf{x}_i), y_i)$$

$$J(f) = -\frac{1}{n} \sum_{i=1}^n (y_i \log(f(\mathbf{x}_i)) + (1 - y_i) \log(1 - f(\mathbf{x}_i)))$$

Learning

Find the model with the minimal error:

$$\hat{f} = \arg \min_{f \in \mathcal{F}} J(f)$$

Gradient descent

Cost function:

$$J(f) = -\frac{1}{n} \sum_{i=1}^n (y_i \log(f(\mathbf{x}_i)) + (1 - y_i) \log(1 - f(\mathbf{x}_i)))$$

Partial derivate:

$$\frac{\partial J}{\partial w_j} = -\frac{1}{n} \sum_{i=1}^n (y_{i,j} - f(\mathbf{x}_i)) \cdot x_{i,j}$$

Update of a and b :

$$w_j \leftarrow w_j - \eta \frac{\partial J}{\partial w_j}$$

Input variables: $x = \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix}$

Input features

Output: y

Model: $f, y = f(x)$

The "artificial intelligence"

Loss: $l(f(x), y)$

Quantifies how much the prediction is far from the true output

Cost function: $J(f) = \frac{1}{n} \sum_{i=1}^n l(f(x_i), y_i)$

Quantifies how much the prediction is far from the true output across all training examples

Learning: $\hat{f} = \arg \min_{f \in \mathcal{F}} J(f)$

Find the model with the minimal error

Gradient descent: $w \leftarrow w - \eta \frac{\partial J}{\partial w}$

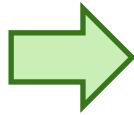
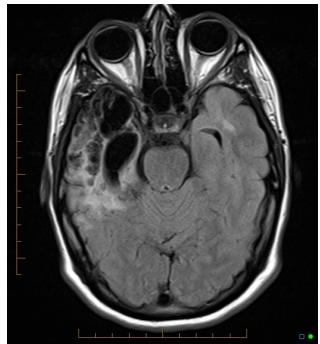
Method to find the model with the minimal error

ML vs DL : learning features

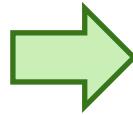
ML

Feature extraction

Classification



Hand-crafted



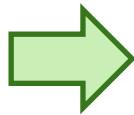
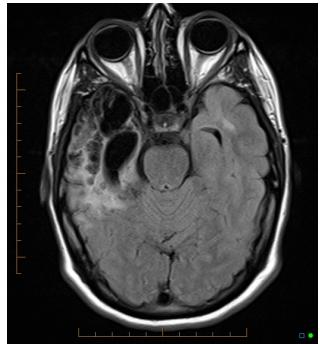
Machine learning



Glioblastoma

Herpes simplex encephalitis

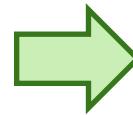
DL



Machine learning



Machine learning

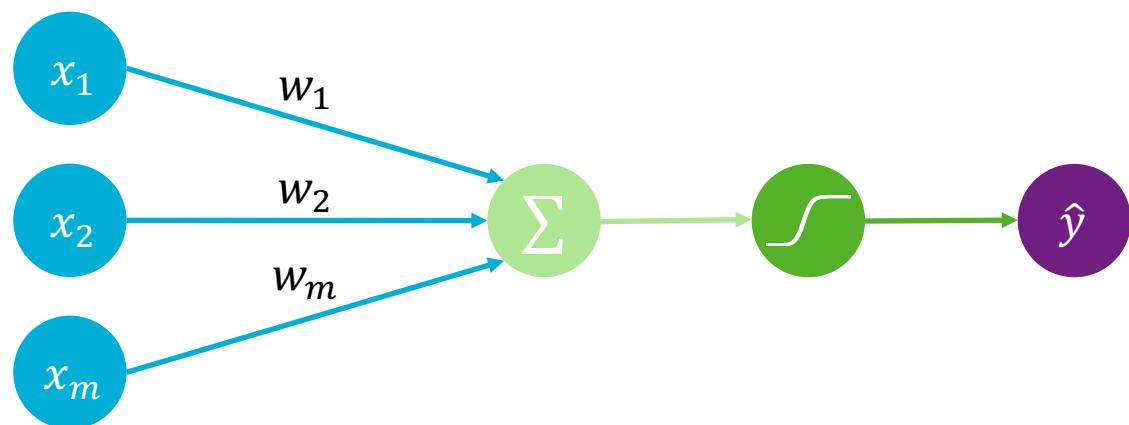


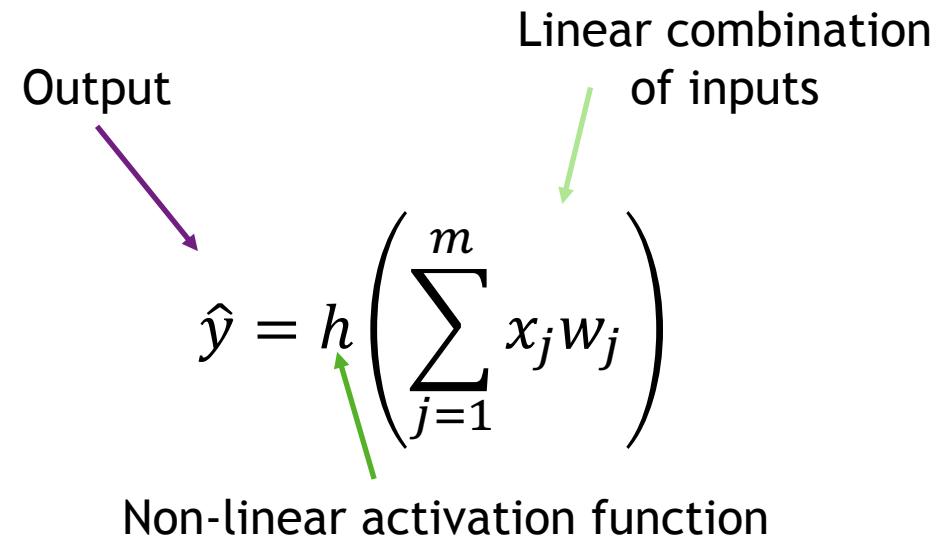
Glioblastoma

Herpes simplex encephalitis

Neural networks

Artificial neuron





The equation for the output of an artificial neuron is:

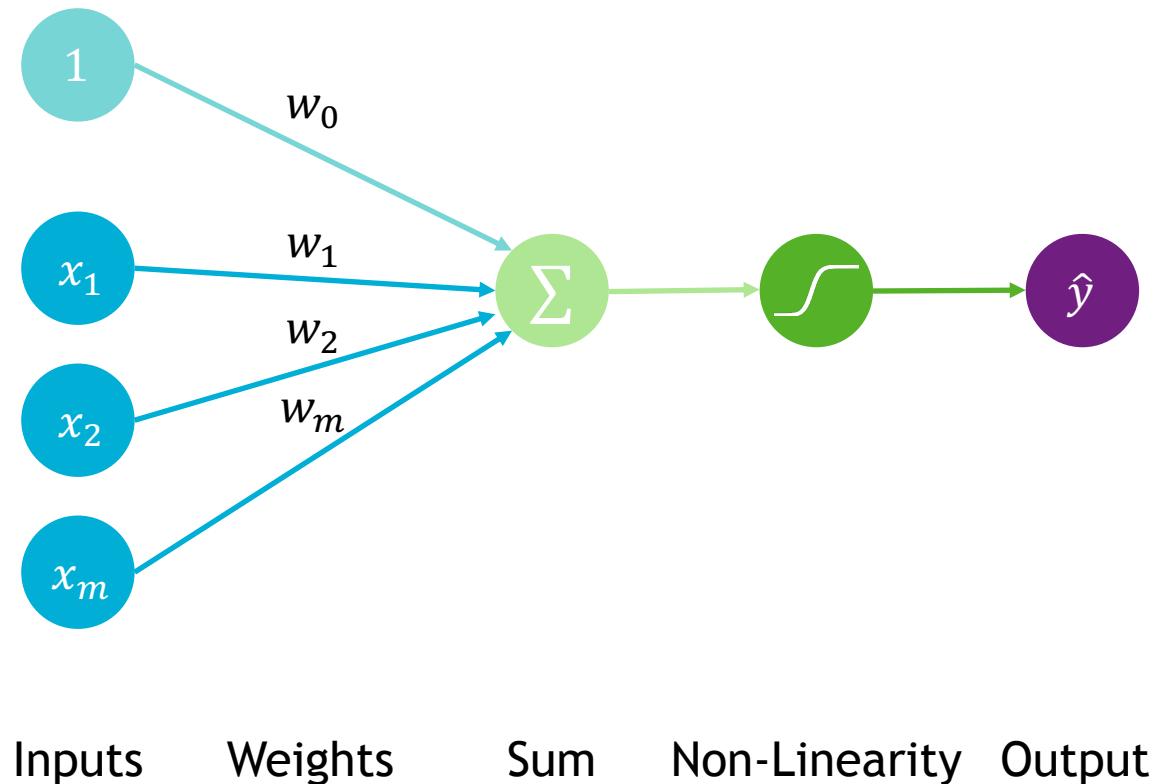
$$\hat{y} = h\left(\sum_{j=1}^m x_j w_j\right)$$

Annotations explain the components:

- Output: Points to the purple circle \hat{y} .
- Linear combination of inputs: Points to the term $\sum_{j=1}^m x_j w_j$.
- Non-linear activation function: Points to the green circle containing the sigmoid curve.

Inputs Weights Sum Non-Linearity Output

Artificial neuron



Linear combination of inputs

Output

Bias

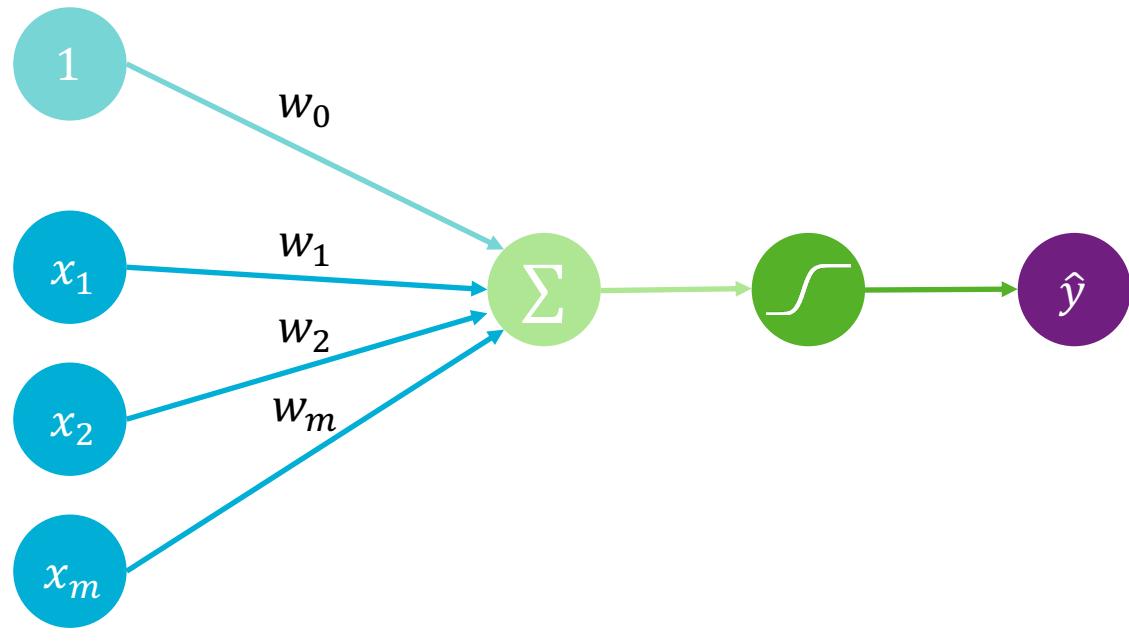
$\hat{y} = h\left(w_0 + \sum_{j=1}^m x_j w_j\right)$

Non-linear activation function

$$\hat{y} = h(w_0 + X^T W)$$

where $X = \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix}$ and $W = \begin{bmatrix} w_1 \\ \vdots \\ w_m \end{bmatrix}$

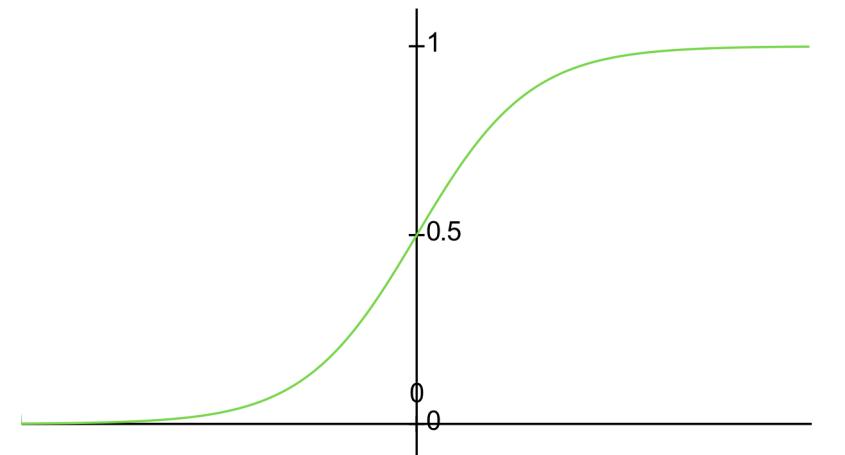
Activation function



Inputs Weights Sum Non-Linearity Output

$$\hat{y} = h(w_0 + \mathbf{X}^T \mathbf{W})$$

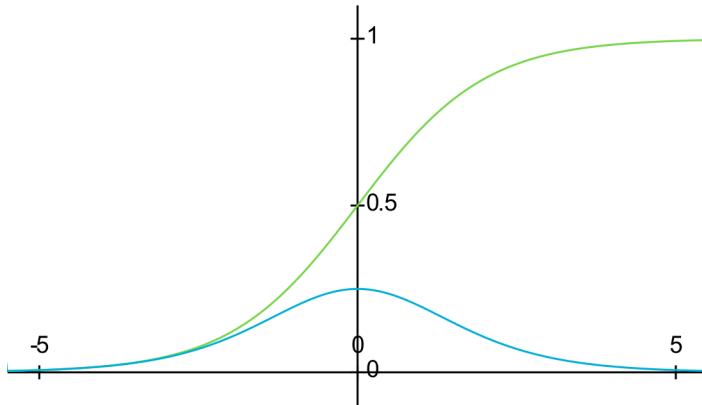
Sigmoid function: $h(z) = \frac{1}{1 + e^{-z}}$



→ Logistic regression

Examples of activation functions

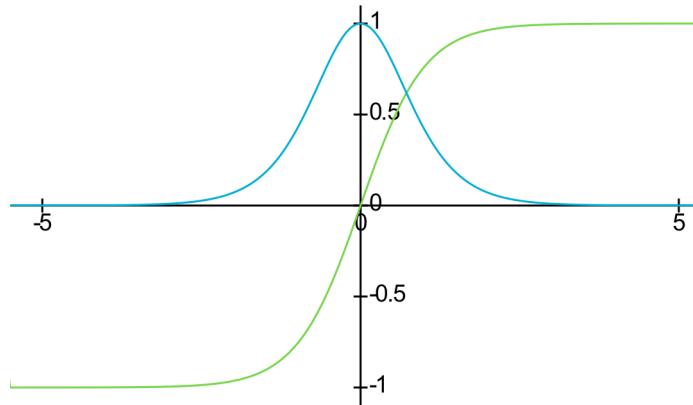
Sigmoid



$$h(z) = \frac{1}{1 + e^{-z}}$$

$$h'(z) = h(z)(1 - h(z))$$

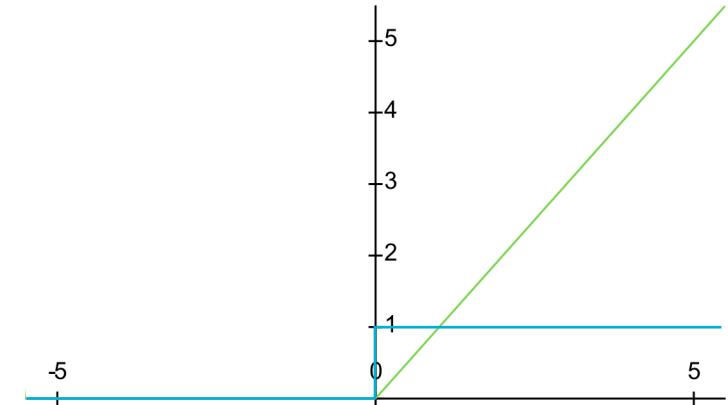
Hyperbolic tangent



$$h(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$$

$$h'(z) = 1 - h(z)^2$$

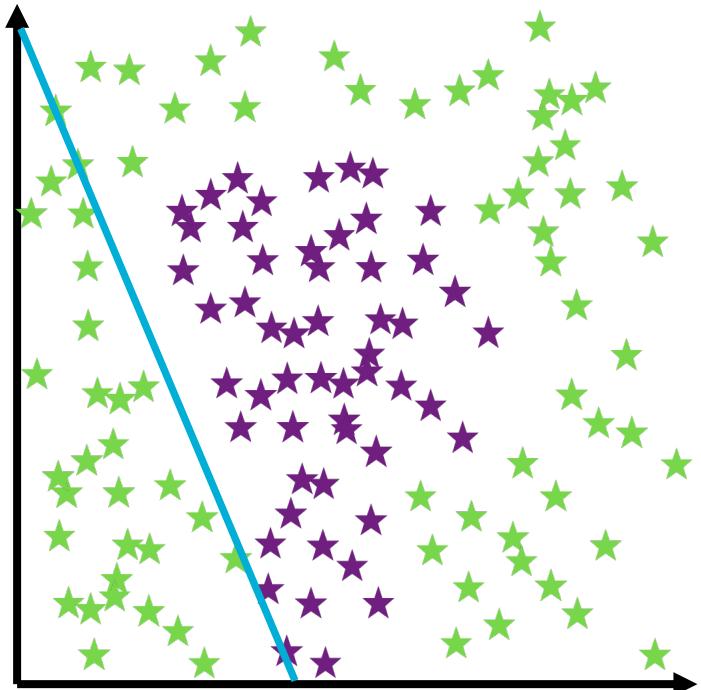
Rectified linear unit (ReLU)



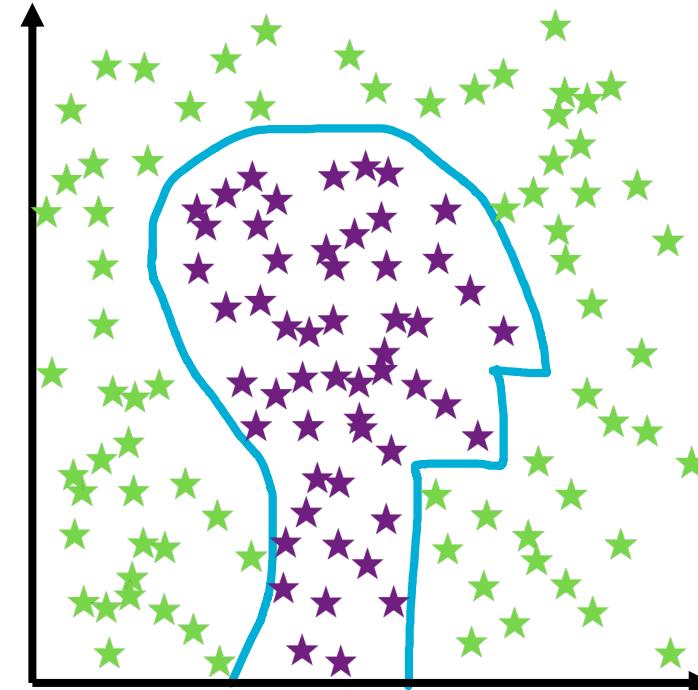
$$h(z) = \max(0, z)$$

$$h'(z) = \begin{cases} 1, & z > 0 \\ 0, & \text{otherwise} \end{cases}$$

Importance of non-linear activation functions

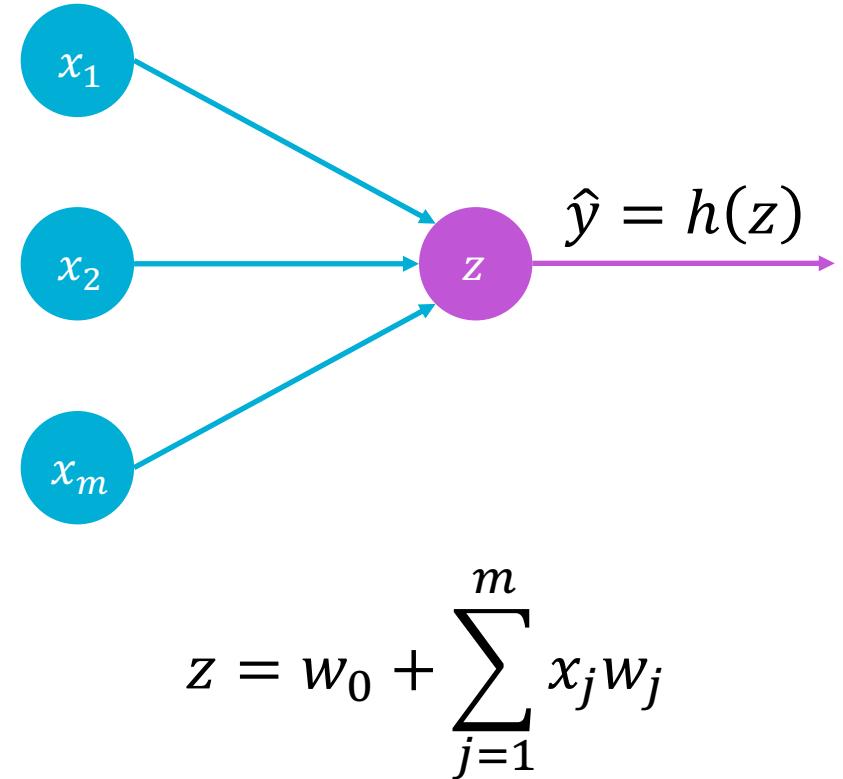
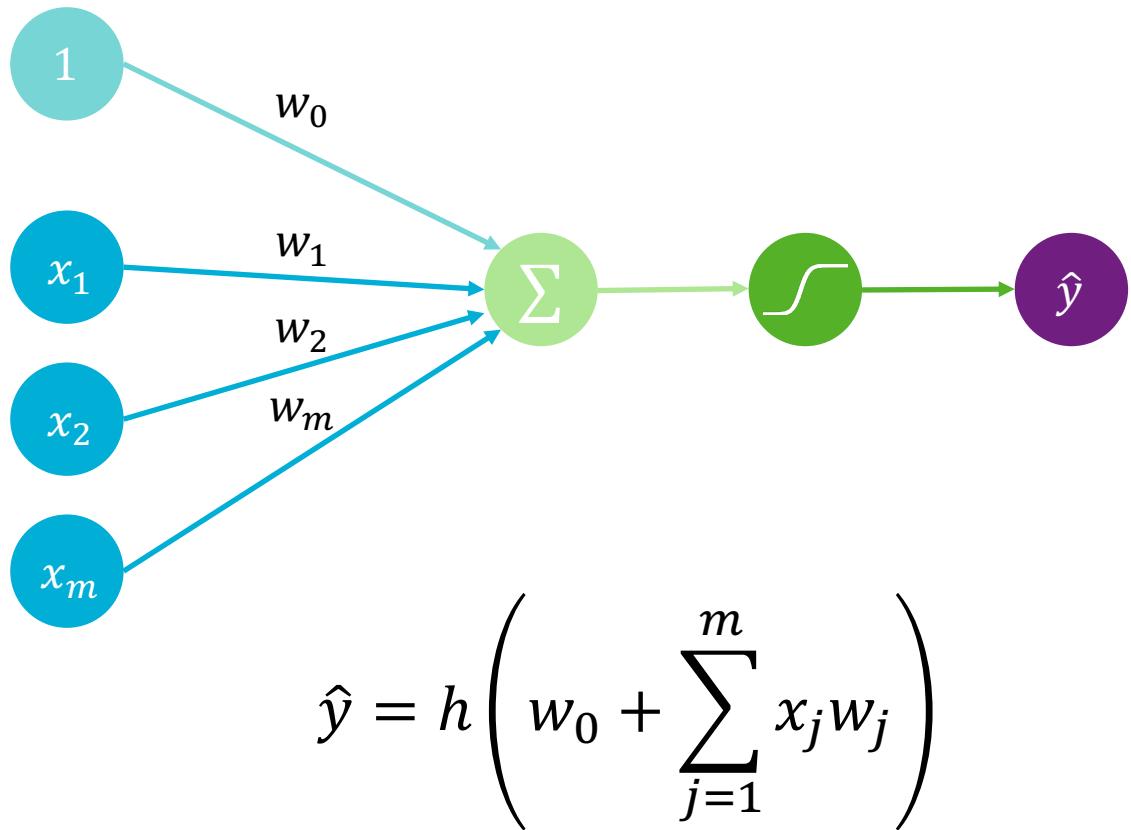


Linear activation functions
→ linear decisions

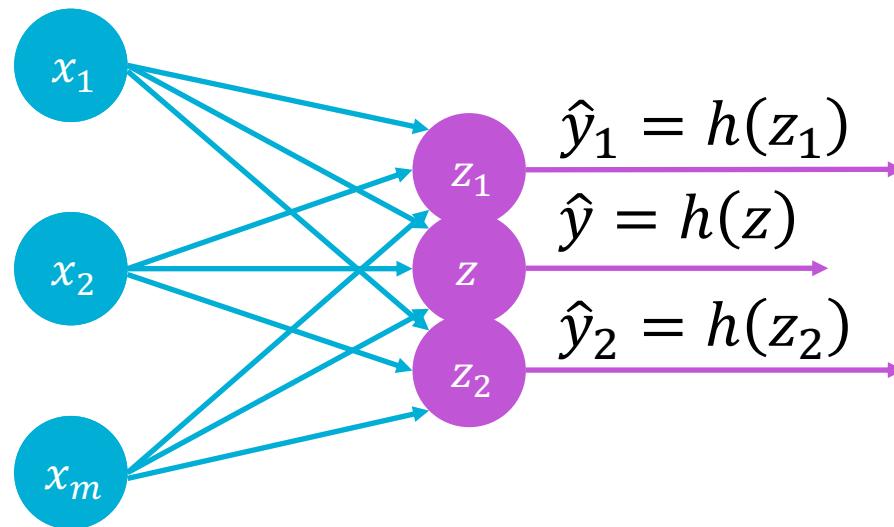


Non-linear activation functions
→ arbitrarily complex decisions

Simplified notation

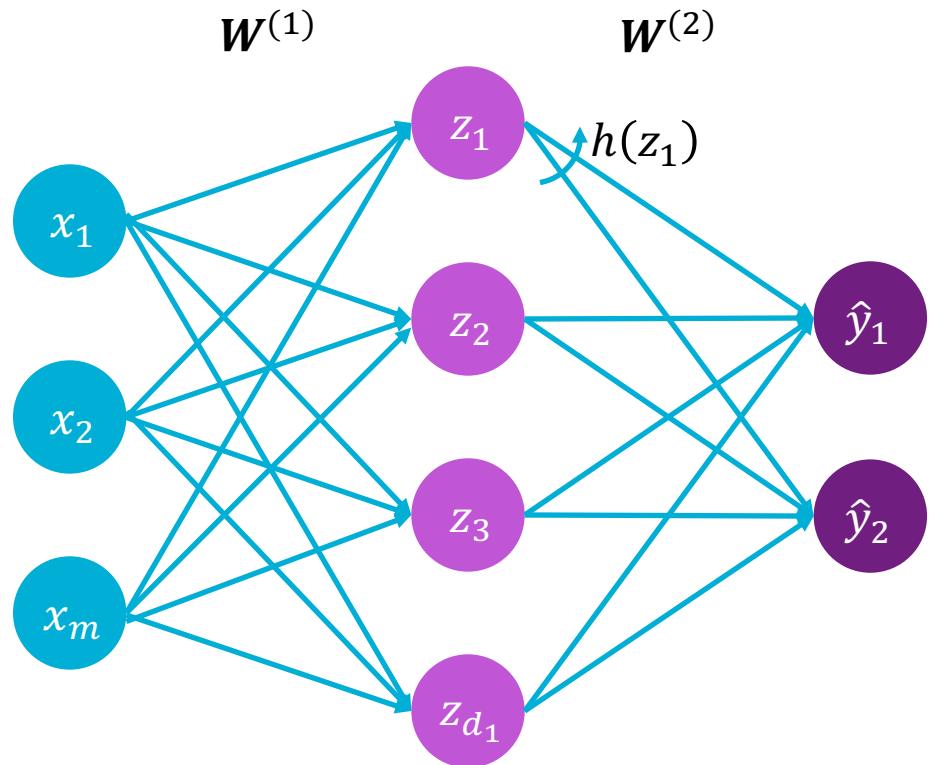


Multi output neural network with dense layers



$$z_i = w_{0,i} + \sum_{j=1}^m x_j w_{j,i}$$

Single layer neural network



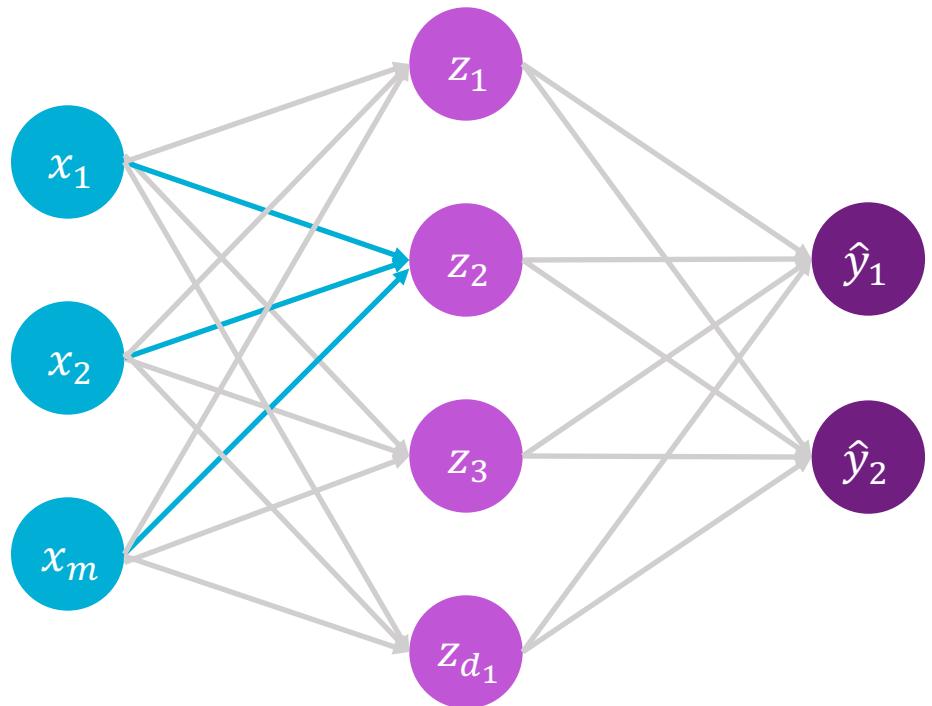
Inputs

Hidden

Output

$$z_i = w_{0,i}^{(1)} + \sum_{j=1}^m x_j w_{j,i}^{(1)}$$
$$\hat{y}_i = h\left(w_{0,i}^{(2)} + \sum_{j=1}^{d_1} z_j w_{j,i}^{(2)}\right)$$

Single layer neural network



Inputs

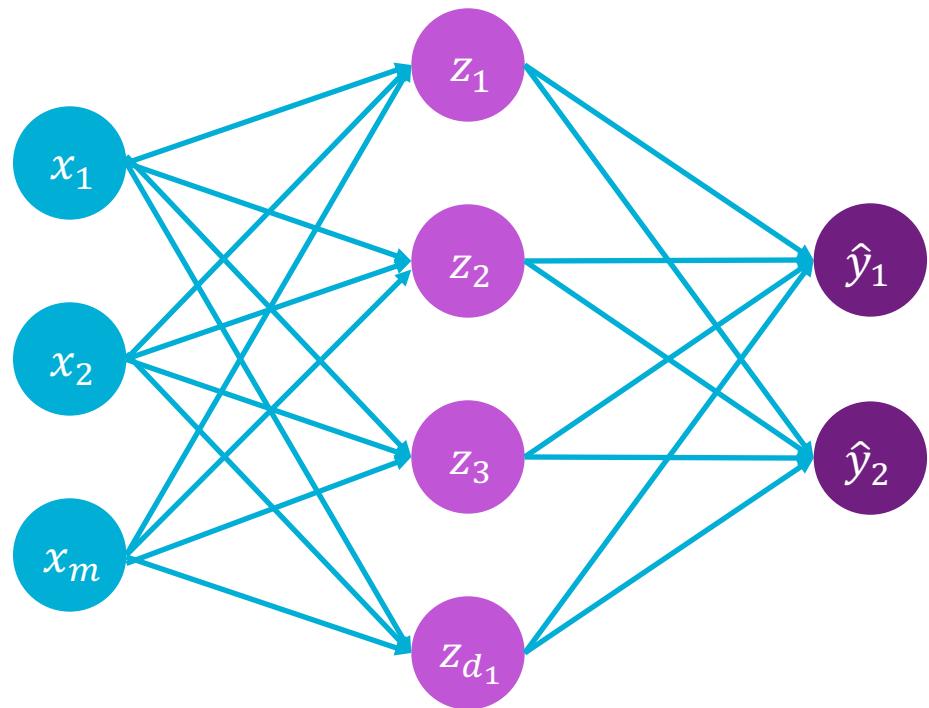
Hidden

Output

$$\begin{aligned} z_2 &= w_{0,2}^{(1)} + \sum_{j=1}^m x_j w_{j,2}^{(1)} \mathbf{x} \\ &= w_{0,2}^{(1)} + x_1 w_{1,2}^{(1)} + x_2 w_{2,2}^{(1)} + x_m w_{m,2}^{(1)} \end{aligned}$$

Single layer neural network

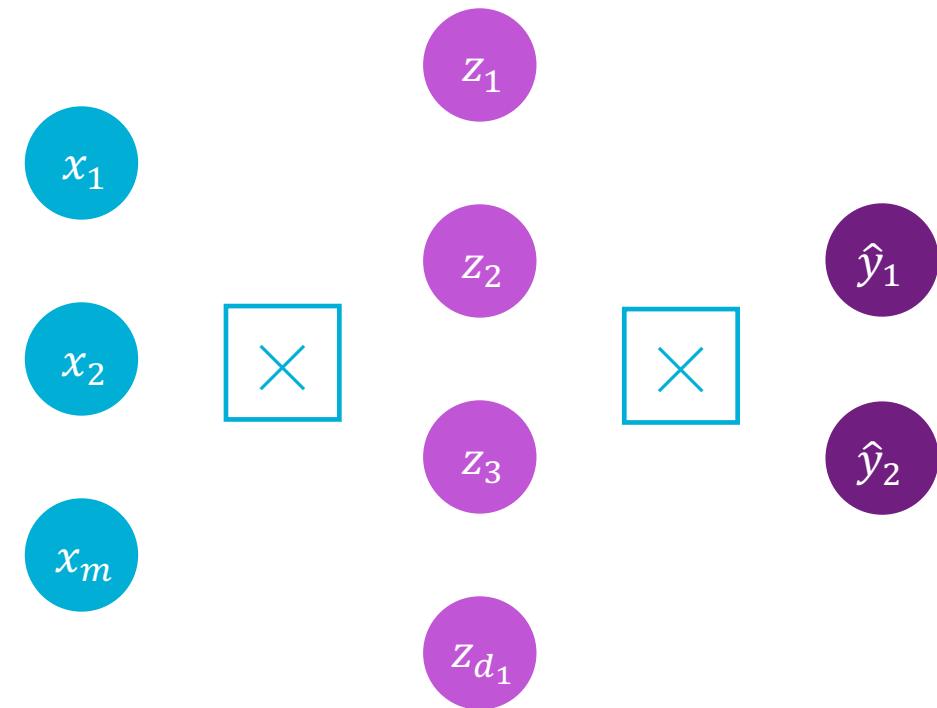
Simplified notation



Inputs

Hidden

Output

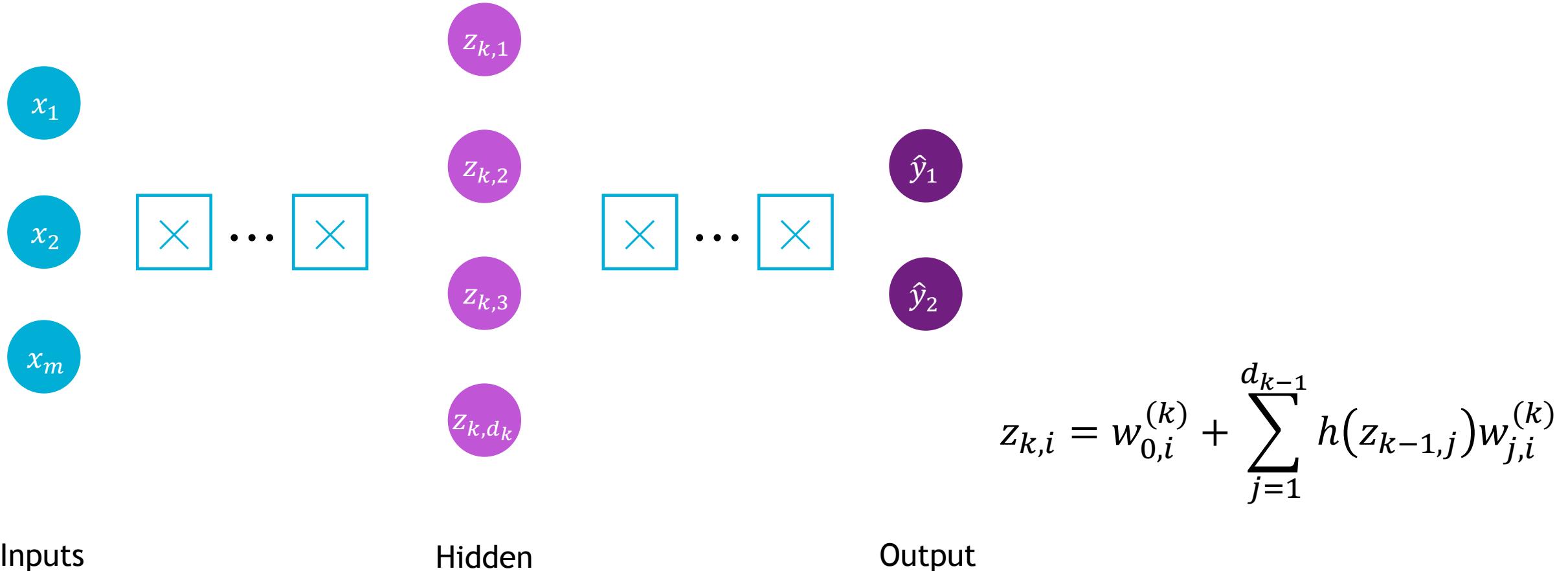


Inputs

Hidden

Output

Stacking layers



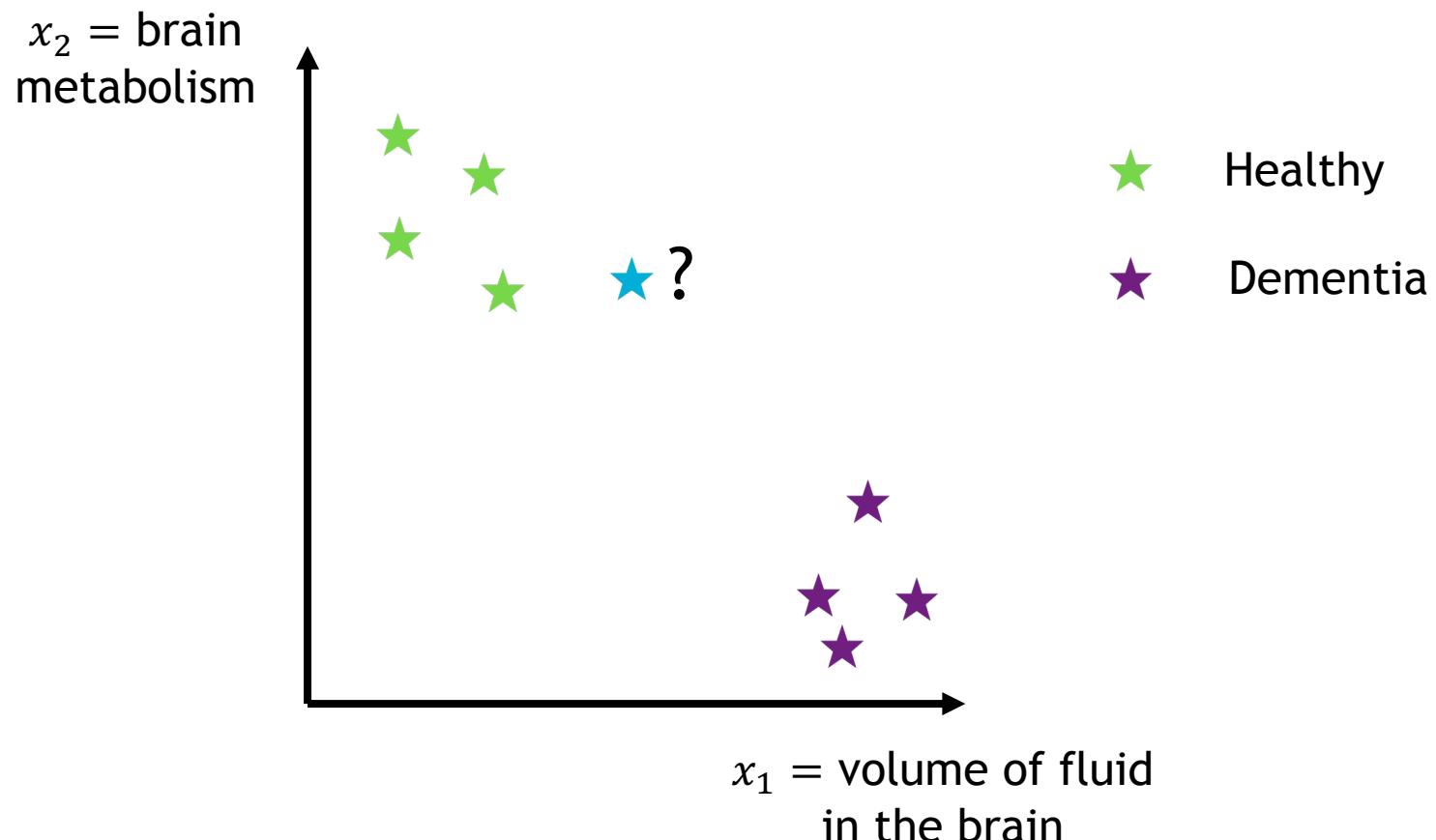
Inputs

Hidden

Output

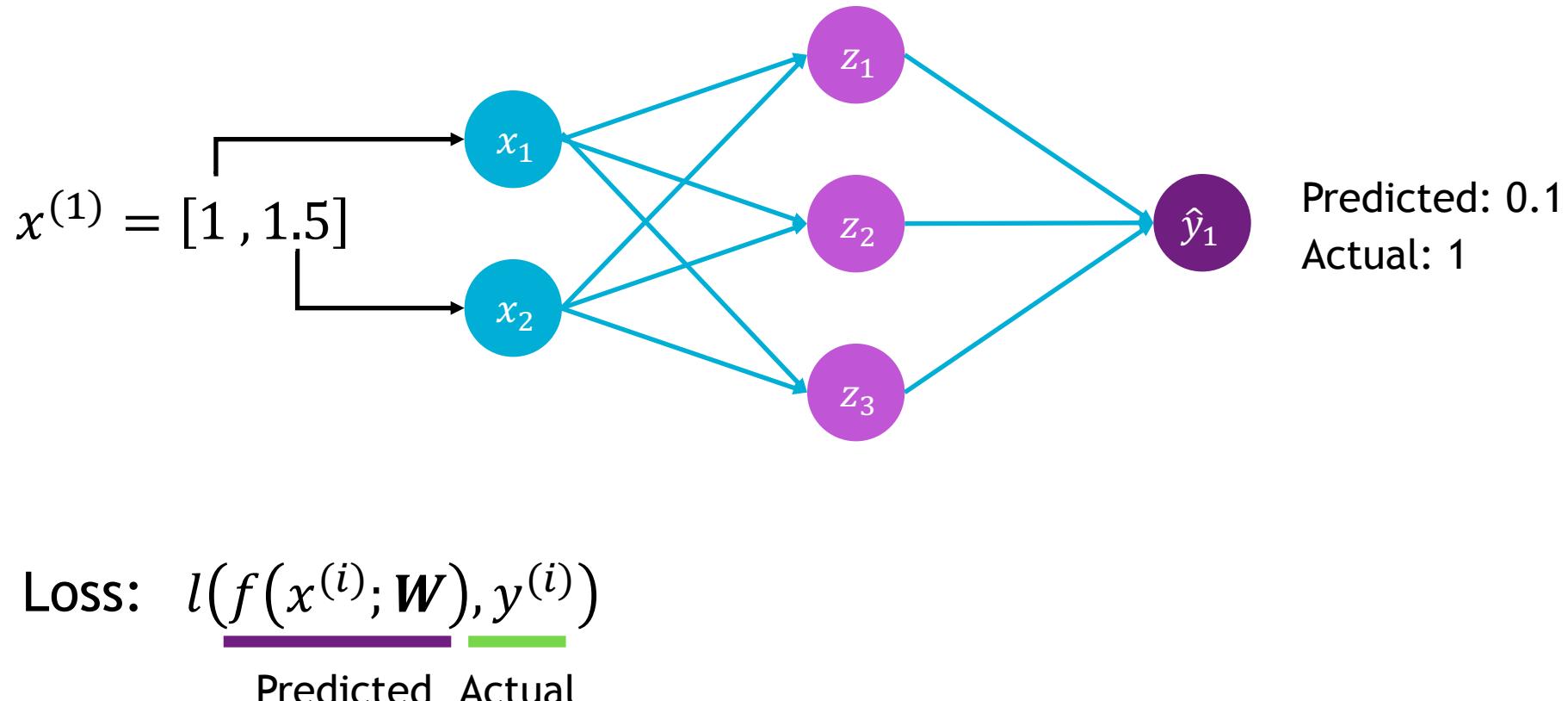
Diagnosis of dementia based on imaging biomarkers

Is this subject healthy?



Diagnosis of dementia based on imaging biomarkers

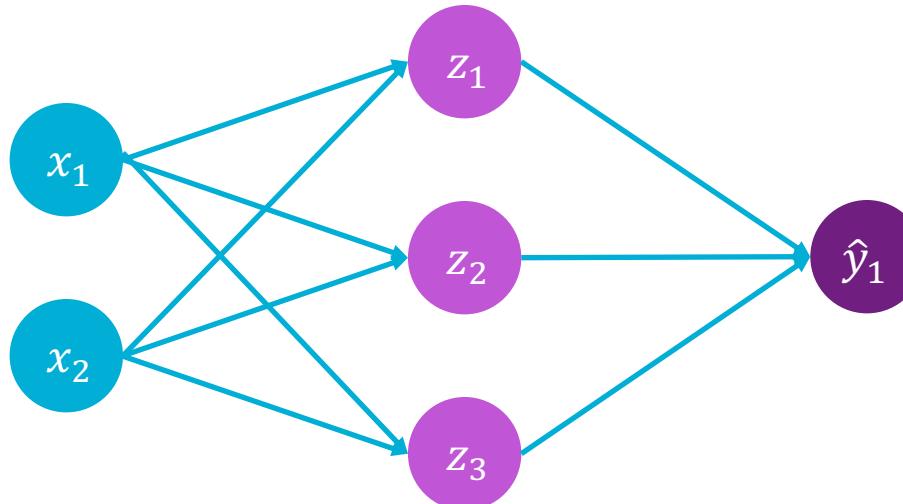
Is this subject healthy?



Diagnosis of dementia based on imaging biomarkers

Is this subject healthy?

$$X = \begin{bmatrix} 1 & 1.5 \\ 3.5 & 1.2 \\ 5 & 0.9 \\ \vdots & \vdots \end{bmatrix}$$



$$\begin{array}{c} f(x) \\ \left[\begin{array}{c} 0.1 \\ 0.4 \\ 0.6 \\ \vdots \end{array} \right] \\ \hline \text{Predicted} \end{array} \quad \begin{array}{c} y \\ \left[\begin{array}{c} 1 \\ 0 \\ 0 \\ \vdots \end{array} \right] \\ \hline \text{Actual} \end{array}$$

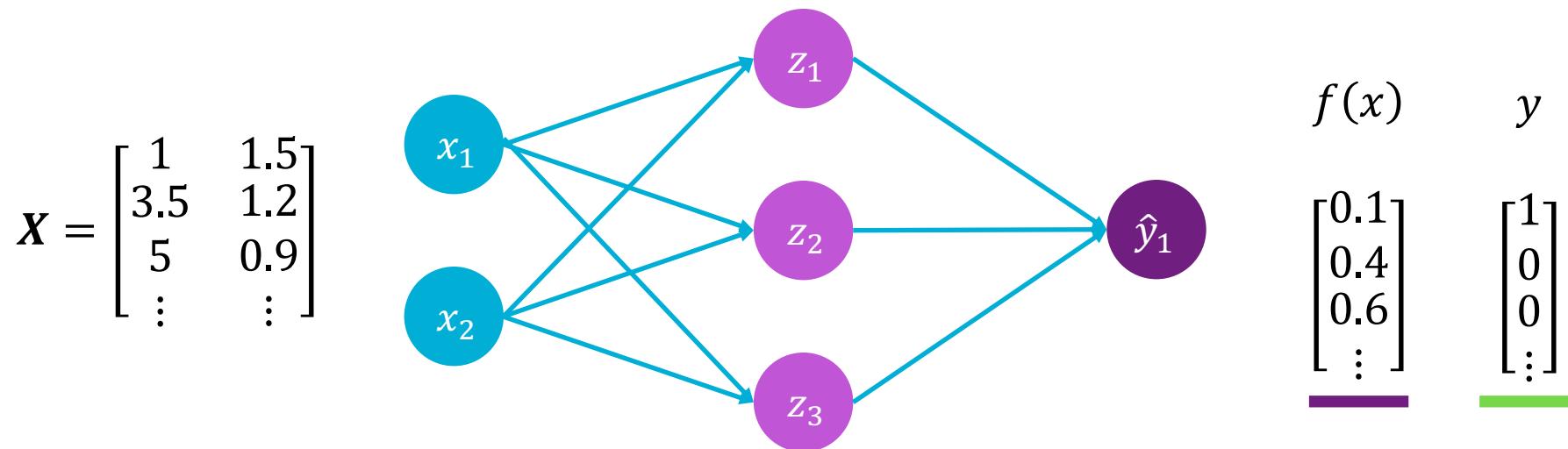
Cost function:

$$J(\mathbf{W}) = \frac{1}{n} \sum_{i=1}^n l(f(x^{(i)}; \mathbf{W}), y^{(i)})$$

Predicted Actual

Diagnosis of dementia based on imaging biomarkers

Is this subject healthy?



Cost function with cross entropy loss:

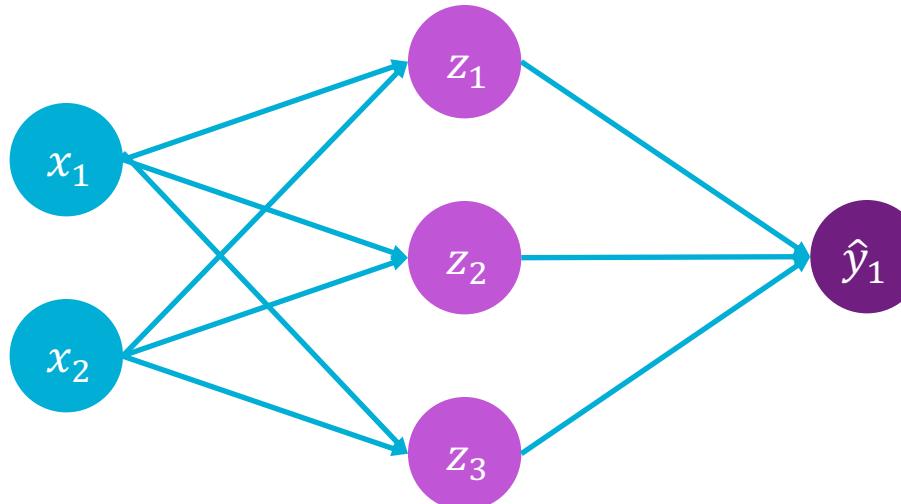
$$J(\mathbf{W}) = \frac{1}{n} \sum_{i=1}^n -\underline{y^{(i)}} \log(\underline{f(x^{(i)}; \mathbf{W})}) - (1 - \underline{y^{(i)}}) \log(1 - \underline{f(x^{(i)}; \mathbf{W})})$$

Actual Predicted Actual Predicted

Diagnosis of dementia based on imaging biomarkers

What is the dementia severity?

$$X = \begin{bmatrix} 1 & 1.5 \\ 3.5 & 1.2 \\ 5 & 0.9 \\ \vdots & \vdots \end{bmatrix}$$



$$\begin{array}{c} f(x) \\ \left[\begin{array}{c} 3 \\ 1 \\ 8 \\ \vdots \end{array} \right] \\ \hline \text{---} \end{array} \quad \begin{array}{c} y \\ \left[\begin{array}{c} 0 \\ 2 \\ 7 \\ \vdots \end{array} \right] \\ \hline \text{---} \end{array}$$

Cost function with mean squared error loss:

$$J(\mathbf{W}) = \frac{1}{n} \sum_{i=1}^n \left(\underbrace{y^{(i)}}_{\text{Actual}} - \underbrace{f(x^{(i)}; \mathbf{W})}_{\text{Predicted}} \right)^2$$

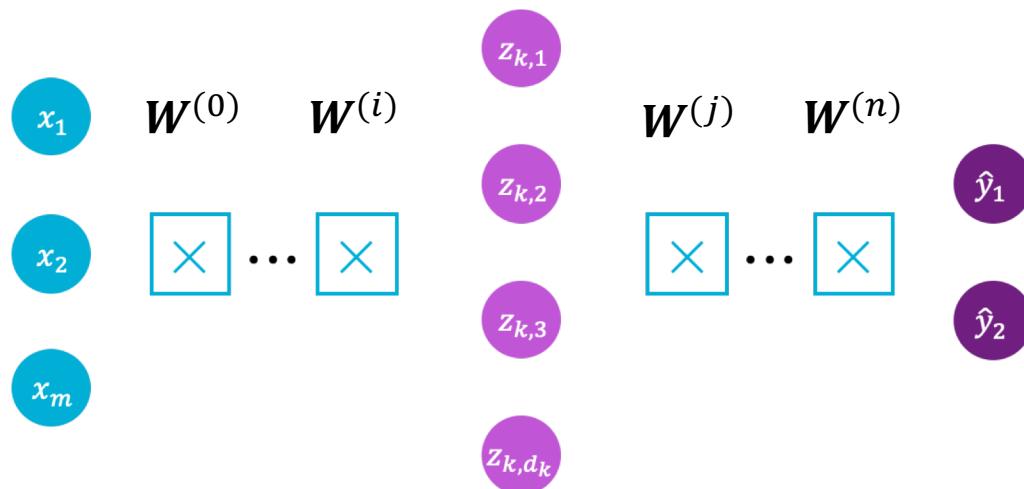
Loss optimisation

- Find the network weights that achieve the lowest loss

$$\mathbf{W}^* = \underset{\mathbf{W}}{\operatorname{argmin}} J(\mathbf{W}) = \underset{\mathbf{W}}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^n l(f(x^{(i)}; \mathbf{W}), y^{(i)})$$

\uparrow

$$\mathbf{W} = \{\mathbf{W}^{(0)}, \mathbf{W}^{(1)}, \dots\}$$



Gradient descent

Algorithm

1. Initialise weights randomly $\sim \mathcal{N}(0, \sigma^2)$
2. Loop until convergence
 - a. Compute gradient $\frac{\partial J(W)}{\partial W}$
 - b. Update weights $W \leftarrow W - \eta \frac{\partial J(W)}{\partial W}$
3. Return weights

Computing gradients: backpropagation



Computing gradients: backpropagation



$$\frac{\partial J(\mathbf{W})}{\partial w_2} = \frac{\partial J(\mathbf{W})}{\partial \hat{y}} \times \frac{\partial \hat{y}}{\partial w_2}$$



Computing gradients: backpropagation



$$\frac{\partial J(\mathbf{W})}{\partial w_2} = \frac{\partial J(\mathbf{W})}{\partial \hat{y}} \times \frac{\partial \hat{y}}{\partial w_2}$$



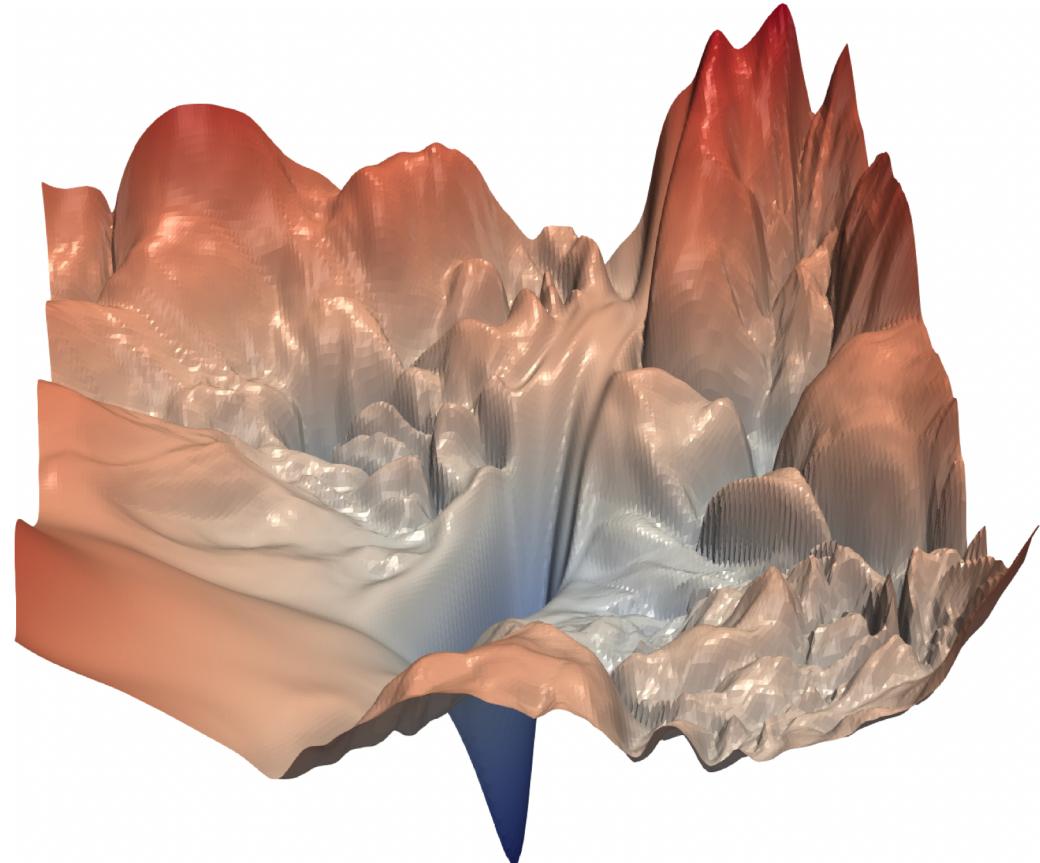
$$\frac{\partial J(\mathbf{W})}{\partial w_1} = \frac{\partial J(\mathbf{W})}{\partial \hat{y}} \times \frac{\partial \hat{y}}{\partial w_1} = \frac{\partial J(\mathbf{W})}{\partial \hat{y}} \times \frac{\partial \hat{y}}{\partial z_1} \times \frac{\partial z_1}{\partial w_1}$$



Gradient descent in practice

Algorithm

1. Initialise weights randomly $\sim \mathcal{N}(0, \sigma^2)$
2. Loop until convergence
 - a. Compute gradient $\frac{\partial J(W)}{\partial W}$
 - b. Update weights $W \leftarrow W - \eta \frac{\partial J(W)}{\partial W}$
3. Return weights

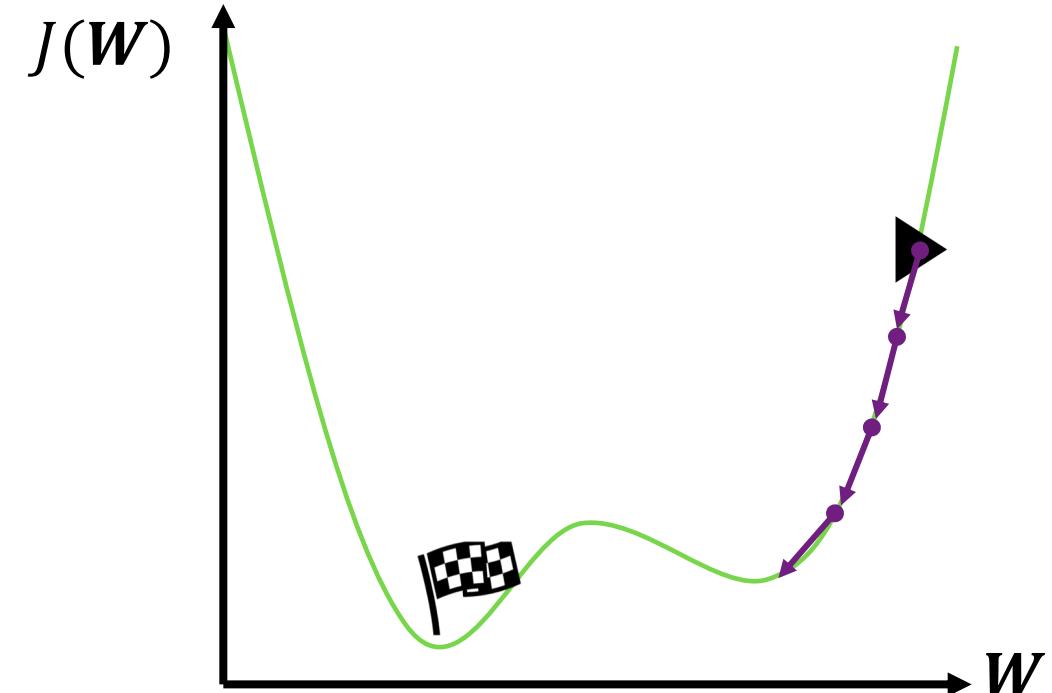


Li et al., Visualizing the Loss Landscape of Neural Nets, NIPS, 2018

Learning rate

$$W \leftarrow W - \eta \frac{\partial J(W)}{\partial W}$$

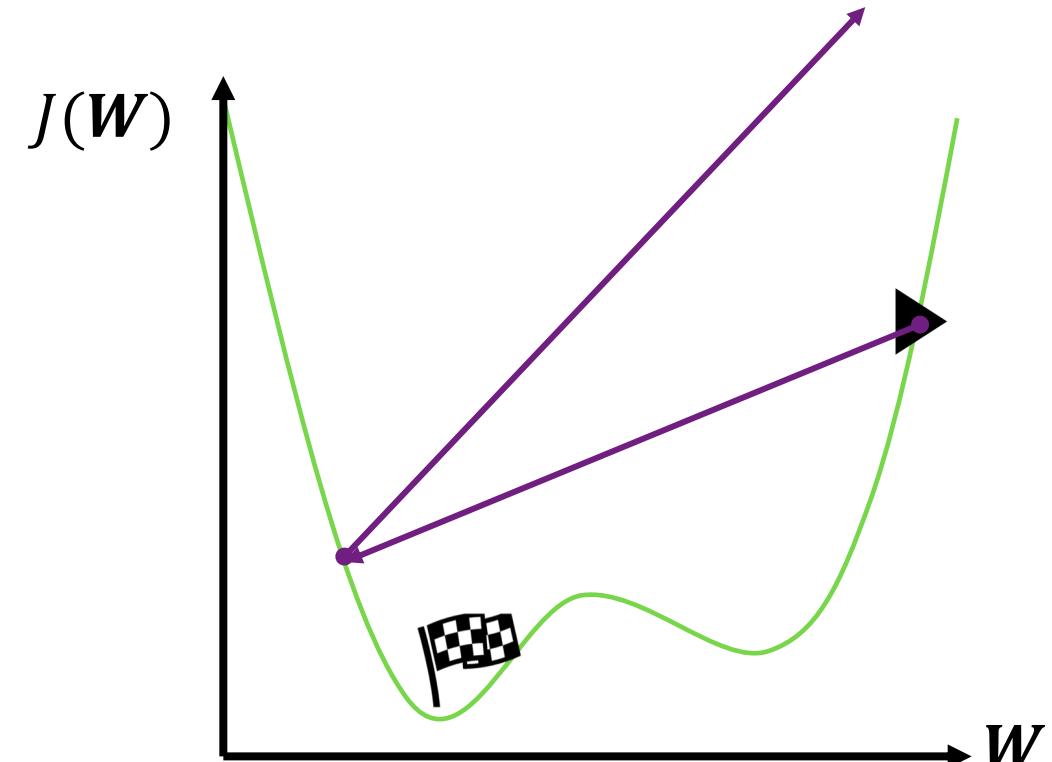
- If η is too small: slow to converge, may be trapped in local minima



Learning rate

$$W \leftarrow W - \eta \frac{\partial J(W)}{\partial W}$$

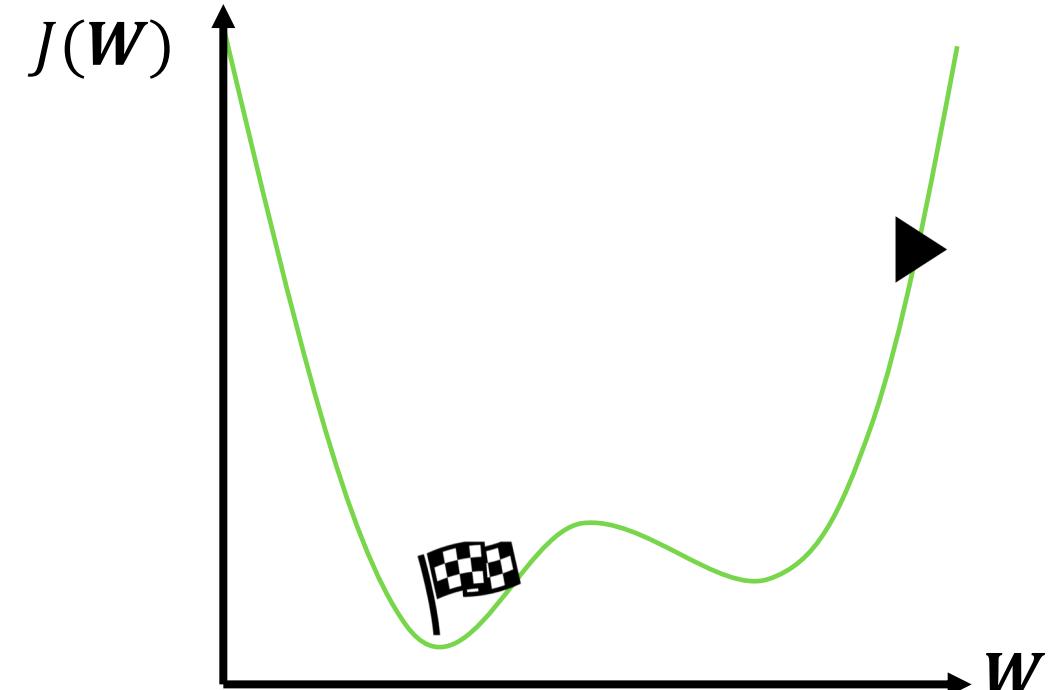
- If η is too small: slow to converge, may be trapped in local minima
- If η is too large: may diverge



Learning rate

$$W \leftarrow W - \eta \frac{\partial J(W)}{\partial W}$$

- If η is too small: slow to converge, may be trapped in local minima
- If η is too large: may diverge



→ Adaptative learning rate

Adaptative learning rate

- Learning rates are no longer fixed
- Can be made larger or smaller depending on:
 - how large the gradient is
 - how fast learning is happening
 - the size of particular weights
 - etc.
- Algorithms:
 - Adam [Kingma et al., Adam: A Method for Stochastic Optimization, 2014]
 - Adadelta [Zeiler et al., ADADELTA: An Adaptive Learning Rate Method, 2012]
 - Adagrad [Duchi et al., Adaptive Subgradient Methods for Online Learning and Stochastic Optimization, 2011]
 - RMSProp [Hinton, Neural Networks for Machine Learning]

Standard gradient descent

Algorithm

1. Initialise weights randomly $\sim \mathcal{N}(0, \sigma^2)$
2. Loop until convergence
 - a. Compute gradient $\frac{\partial J(W)}{\partial W}$ Can be expensive to compute
 - b. Update weights $W \leftarrow W - \eta \frac{\partial J(W)}{\partial W}$
3. Return weights

Stochastic gradient descent with one sample

Algorithm

1. Initialise weights randomly $\sim \mathcal{N}(0, \sigma^2)$
2. Loop until convergence
 - a. Pick single data point i
 - b. Compute gradient $\frac{\partial J_i(W)}{\partial W}$ Easy to compute but very noisy
 - c. Update weights $W \leftarrow W - \eta \frac{\partial J(W)}{\partial W}$
3. Return weights

Stochastic gradient descent with several samples (mini-batch)

Algorithm

1. Initialise weights randomly $\sim \mathcal{N}(0, \sigma^2)$
2. Loop until convergence

a. Pick batch of B data points

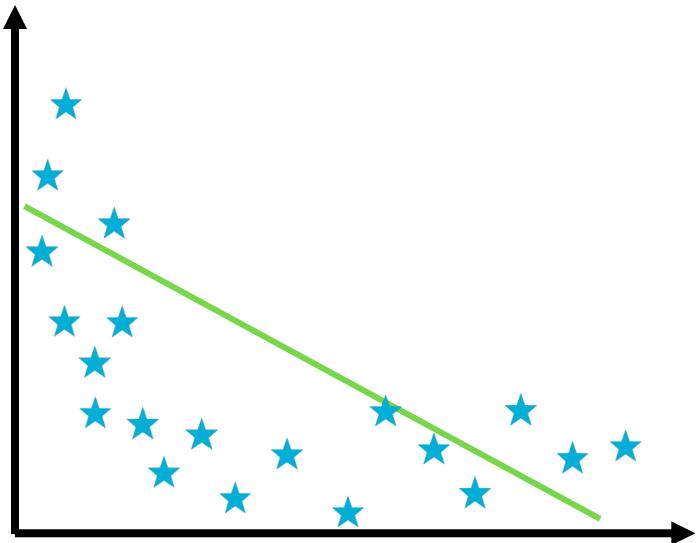
Fast to compute and good estimate of the true gradient

b. Compute gradient
$$\frac{\partial J(\mathbf{W})}{\partial \mathbf{W}} = \frac{1}{B} \sum_{k=1}^B \frac{\partial J_k(\mathbf{W})}{\partial \mathbf{W}}$$

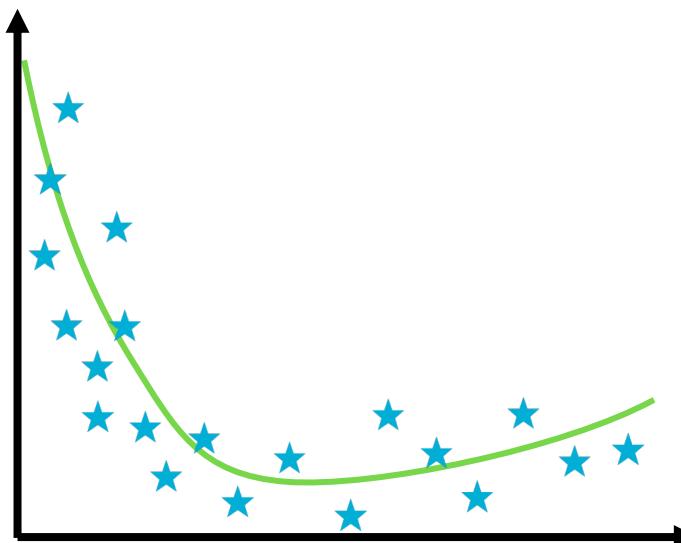
c. Update weights $\mathbf{W} \leftarrow \mathbf{W} - \eta \frac{\partial J(\mathbf{W})}{\partial \mathbf{W}}$

3. Return weights

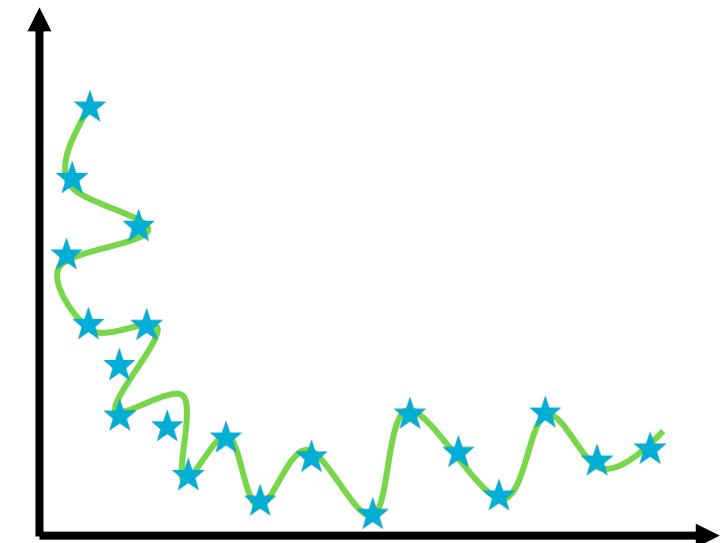
Overfitting



Underfitting

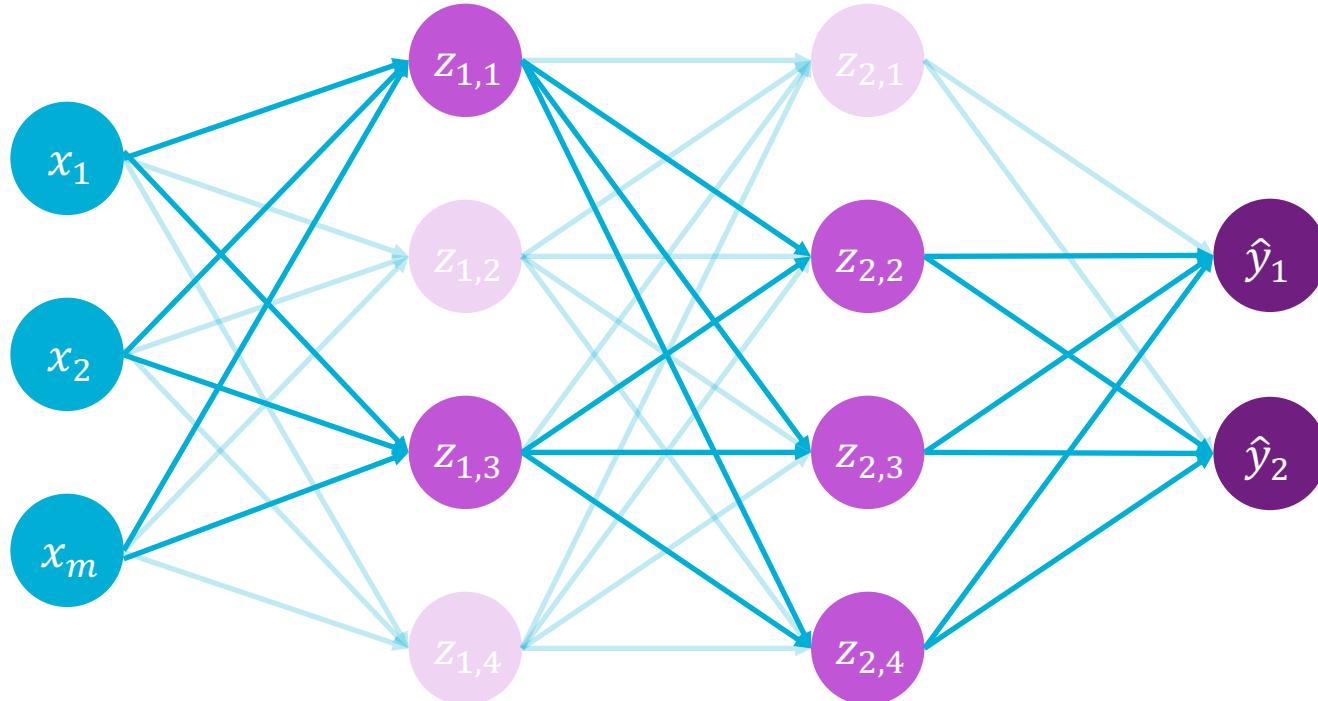


Ideal fit

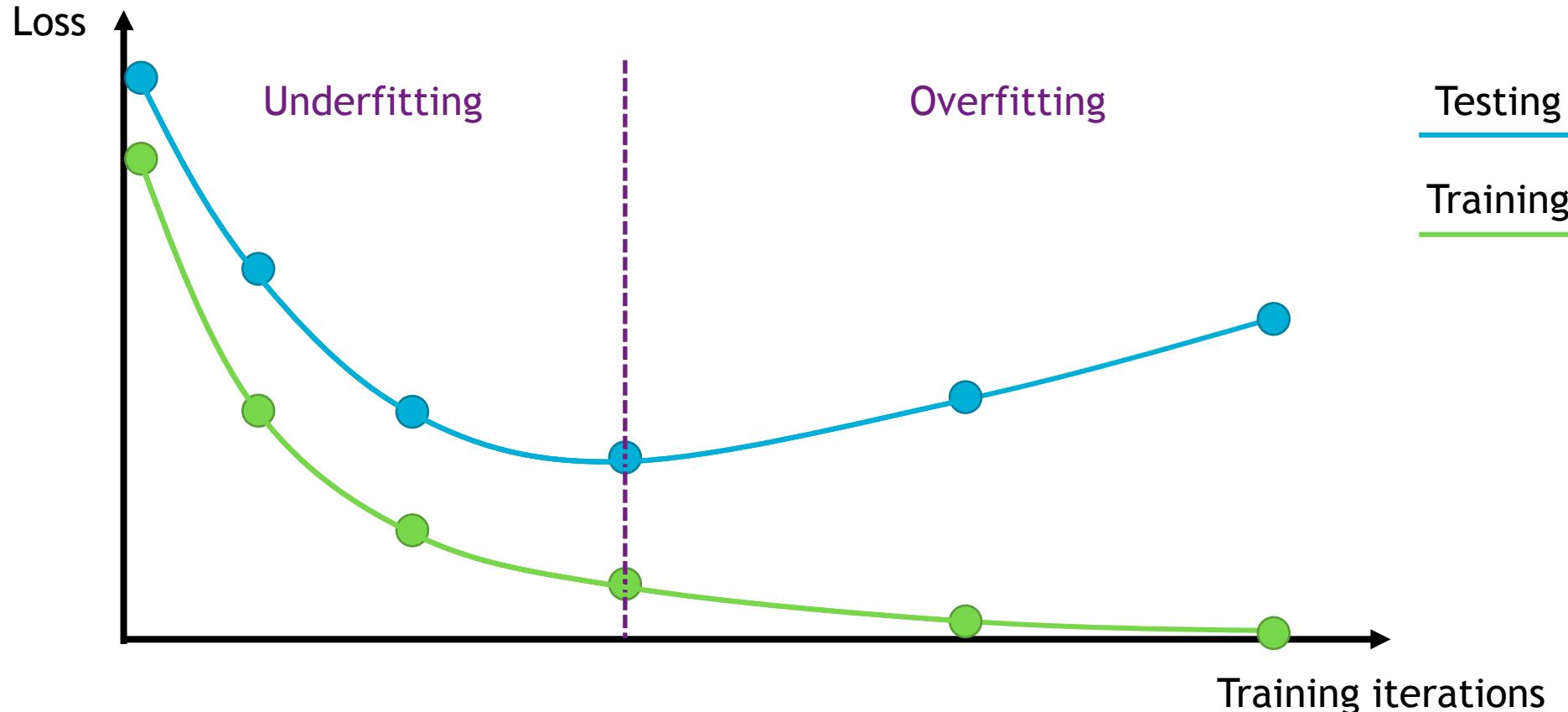


Overfitting

Regularisation: Dropout

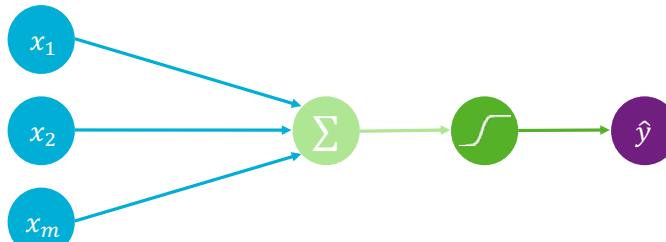


Regularisation: Early stopping



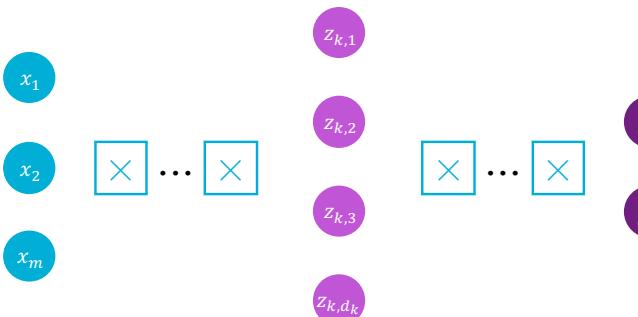
The Perceptron

- Structural building blocks
- Nonlinear activation functions



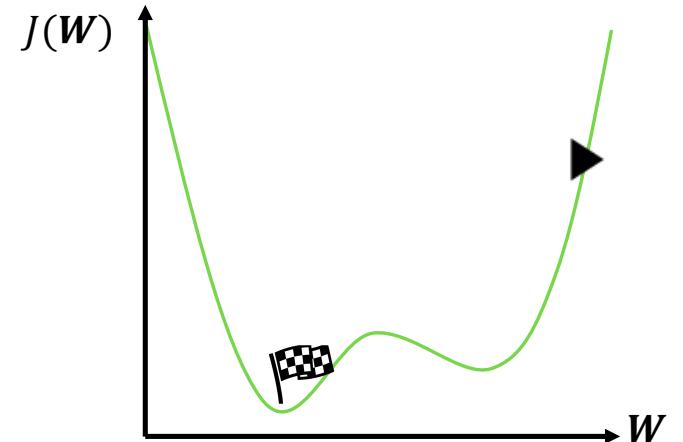
Neural Networks

- Stacking Perceptrons to form neural networks
- Optimisation through backpropagation



Training in Practice

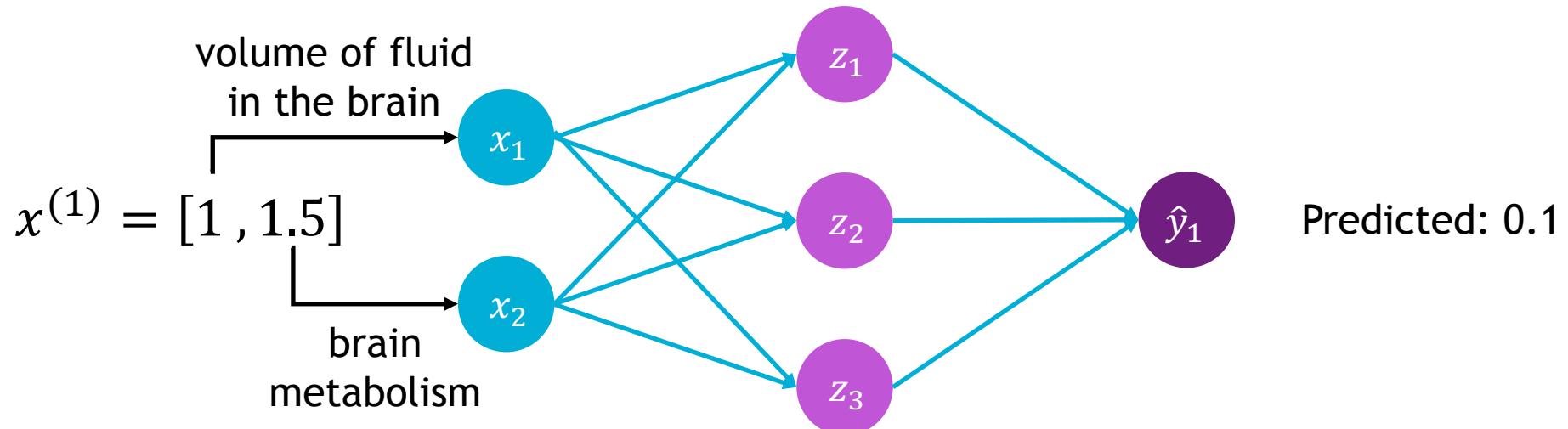
- Adaptive learning
- Batching
- Regularisation



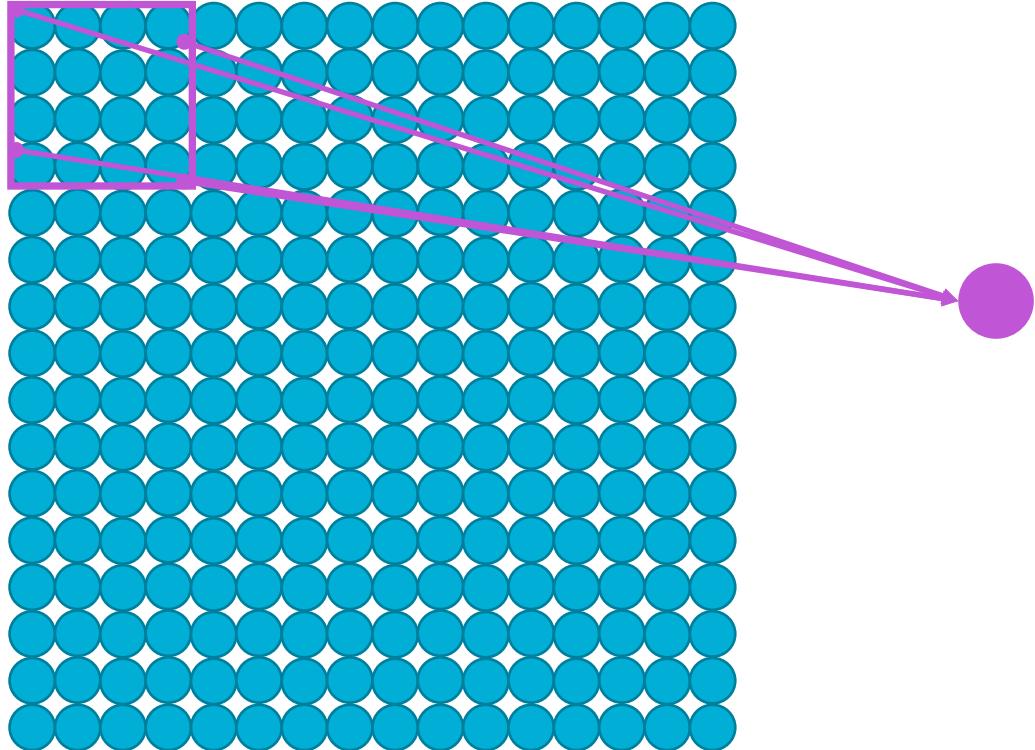
Convolutional neural networks

Diagnosis of dementia based on imaging biomarkers

Is this subject healthy?

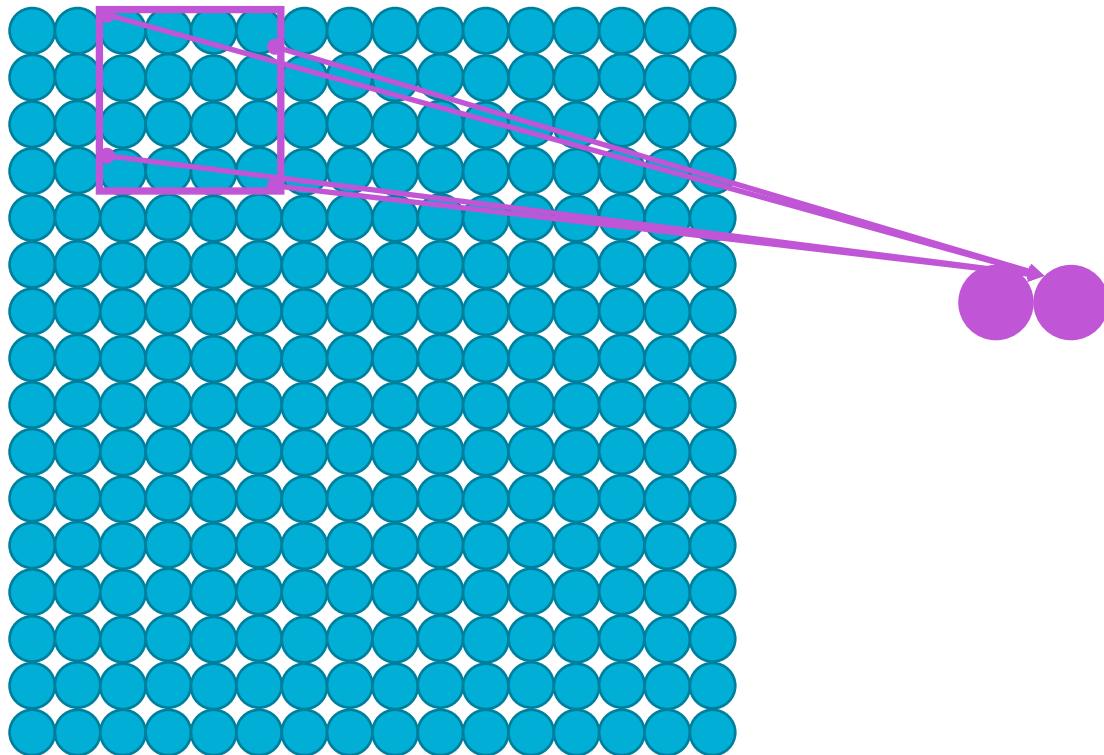


Using spatial features



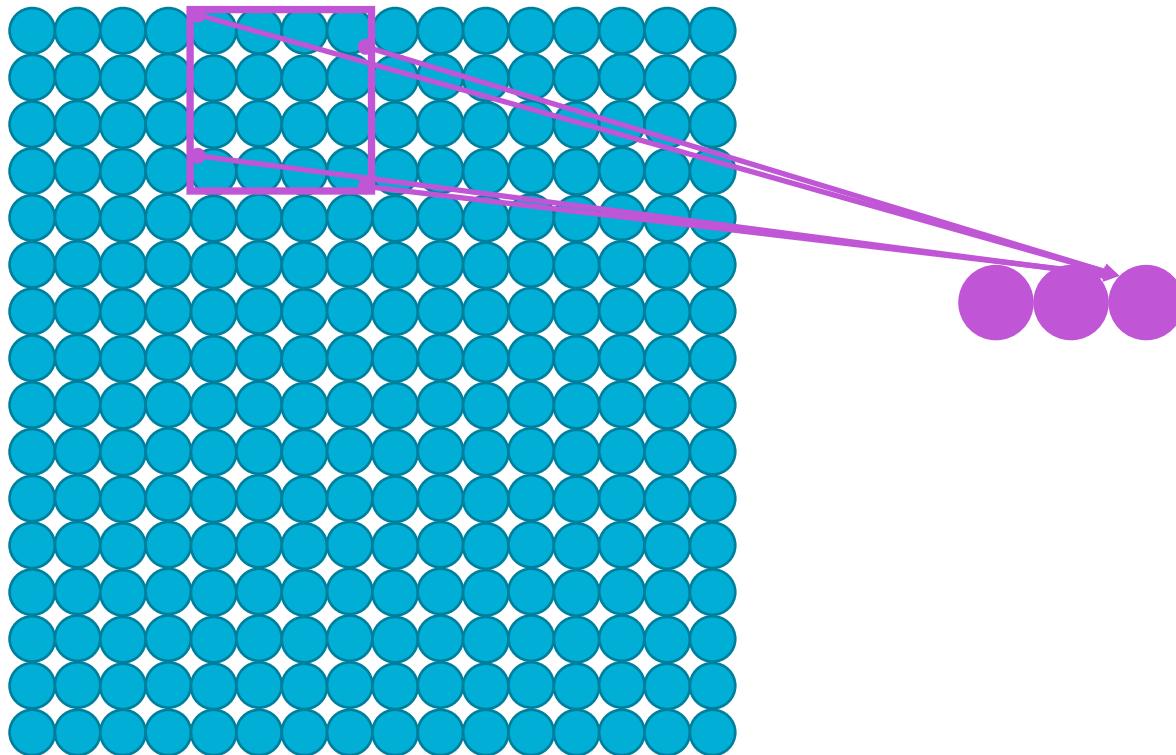
Idea: connect patches of input to neurons in hidden layer

Using spatial features



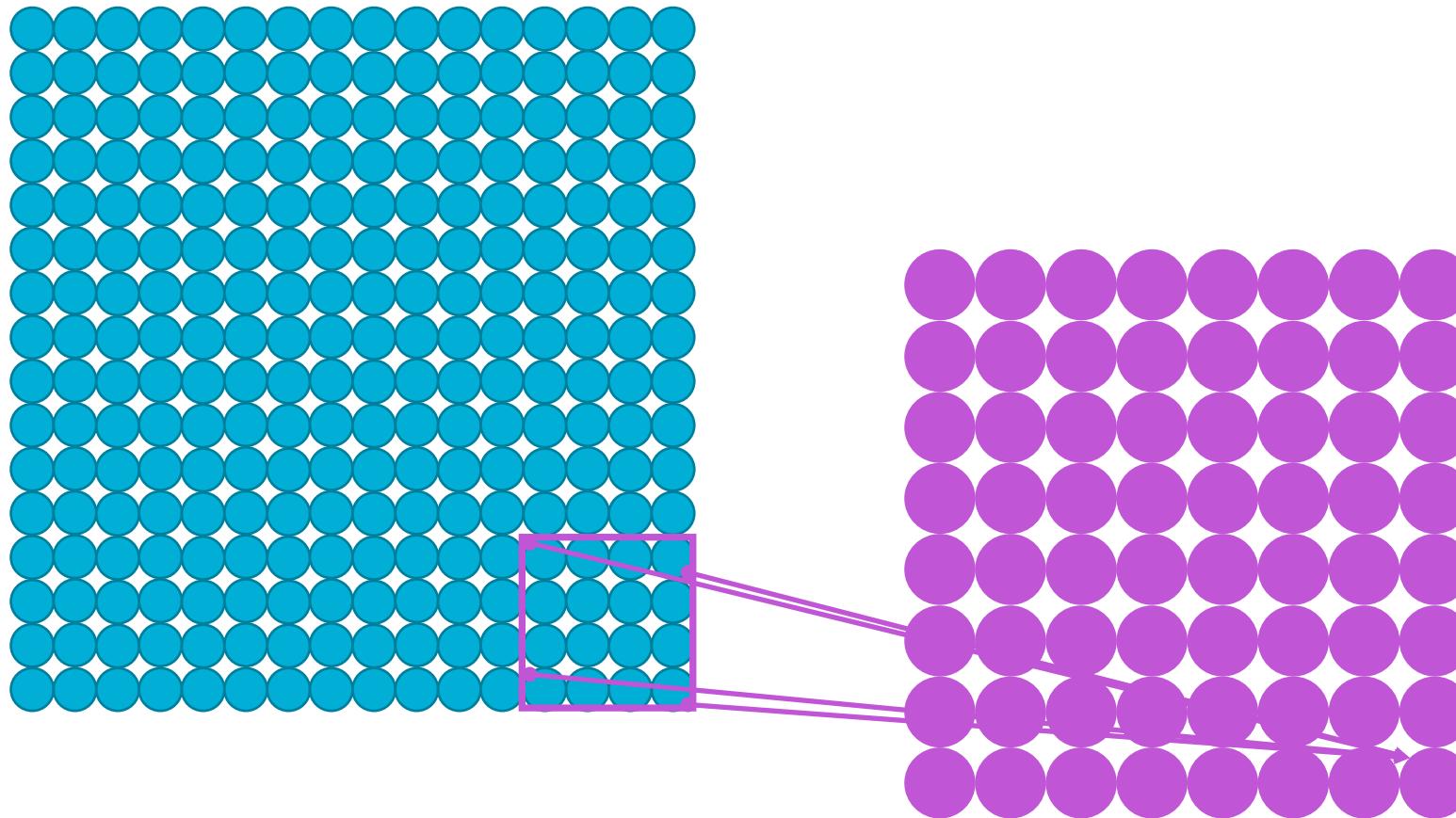
- Slide patch window across input image
 - Weight pixels inside the patch
 - Apply weighted summation
- Convolution

Using spatial features



- Slide patch window across input image
 - Weight pixels inside the patch
 - Apply weighted summation
- Convolution

Using spatial features



- Slide patch window across input image
 - Weight pixels inside the patch
 - Apply weighted summation
- Convolution

The convolution operation

- Slide the filter over the input image
- Element-wise multiply
- Add the outputs

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



Image

1	0	1
0	1	0
1	0	1

Filter

The convolution operation

- Slide the filter over the input image
- Element-wise multiply
- Add the outputs

$$\begin{aligned} & 1 \times 1 + 1 \times 0 + 1 \times 1 \\ & + 0 \times 0 + 1 \times 1 + 1 \times 0 \\ & + 0 \times 1 + 0 \times 0 + 1 \times 1 \\ & = 4 \end{aligned}$$

1×1	1×0	1×1	0	0
0×0	1×1	1×0	1	0
0×1	0×0	1×1	1	1
0	0	1	1	0
0	1	1	0	0



1	0	1
0	1	0
1	0	1

=

4		

Image

Filter

Feature map

The convolution operation

- Slide the filter over the input image
- Element-wise multiply
- Add the outputs

$$\begin{aligned} & 1 \times 1 + 1 \times 0 + 0 \times 1 \\ & + 1 \times 0 + 1 \times 1 + 1 \times 0 \\ & + 0 \times 1 + 1 \times 0 + 1 \times 1 \\ = & 3 \end{aligned}$$

1	1×1	1×0	0×1	0
0	1×0	1×1	1×0	0
0	0×1	1×0	1×1	1
0	0	1	1	0
0	1	1	0	0



Image

1	0	1
0	1	0
1	0	1

Filter

4	3	

Feature map

The convolution operation

- Slide the filter over the input image
- Element-wise multiply
- Add the outputs

$$\begin{aligned}
 & 1 \times 1 + 1 \times 0 + 1 \times 1 \\
 & + 1 \times 0 + 1 \times 1 + 0 \times 0 \\
 & + 1 \times 1 + 0 \times 0 + 0 \times 1 \\
 = & 4
 \end{aligned}$$

1	1	1	0	0
0	1	1	1	0
0	0	1×1	1×0	1×1
0	0	1×0	1×1	0×0
0	1	1×1	0×0	0×1



Image

1	0	1
0	1	0
1	0	1

Filter

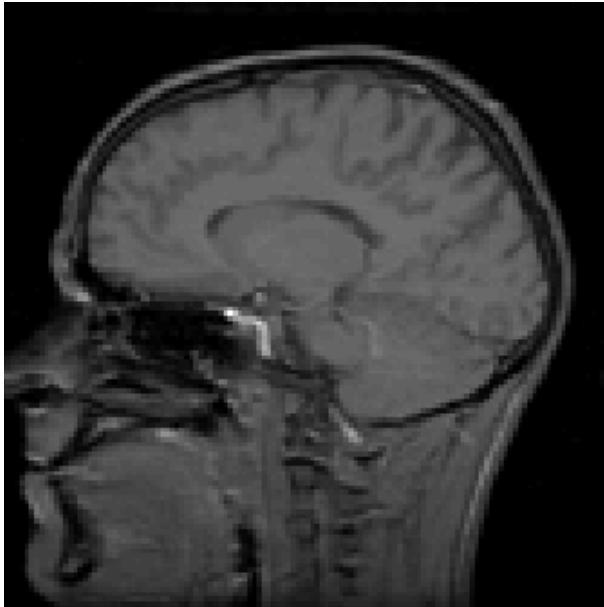
=

4	3	4
2	4	3
2	3	4

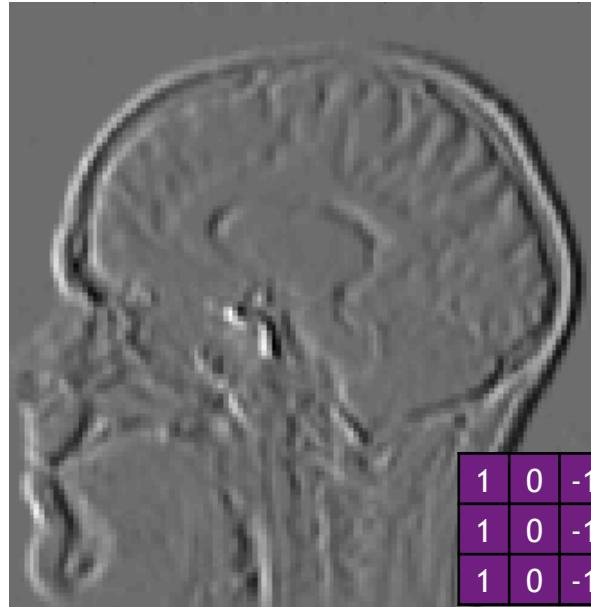
Feature map

Using an image as input of a neural network

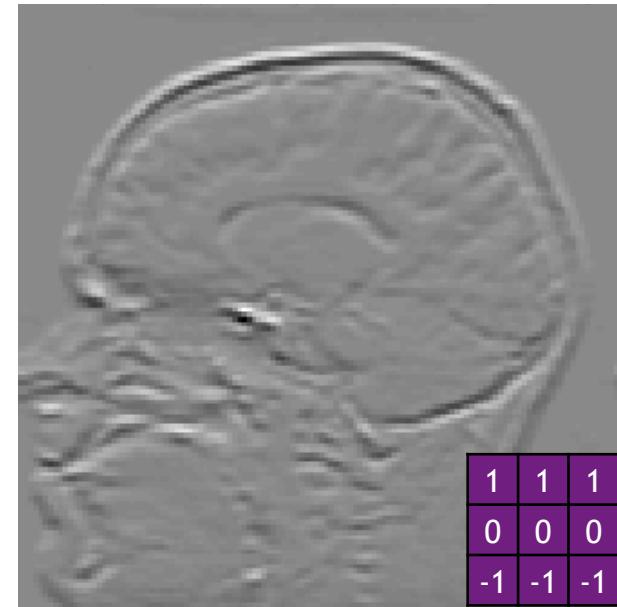
Different filters = different feature maps



Original image

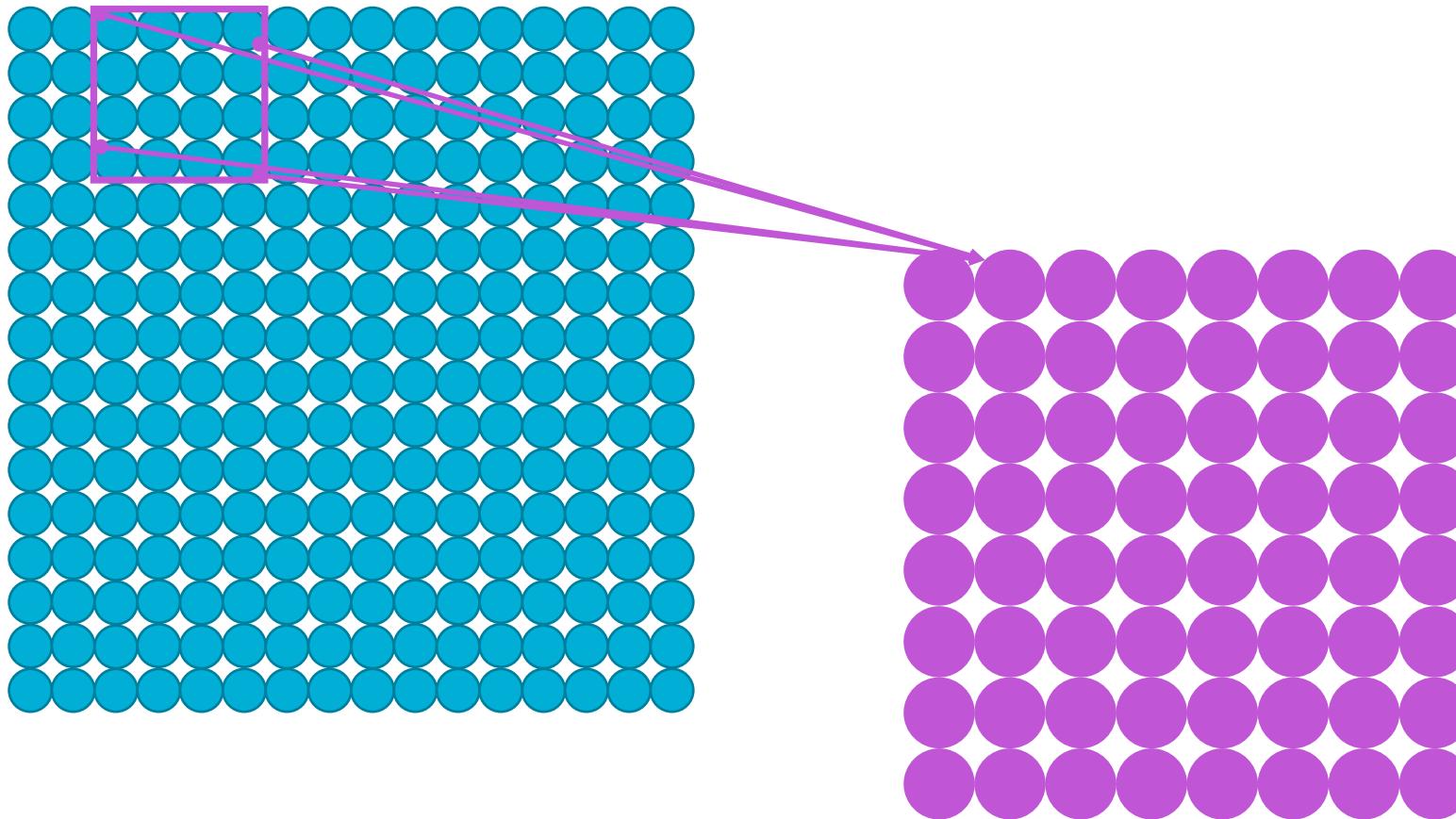


Vertical edge detection



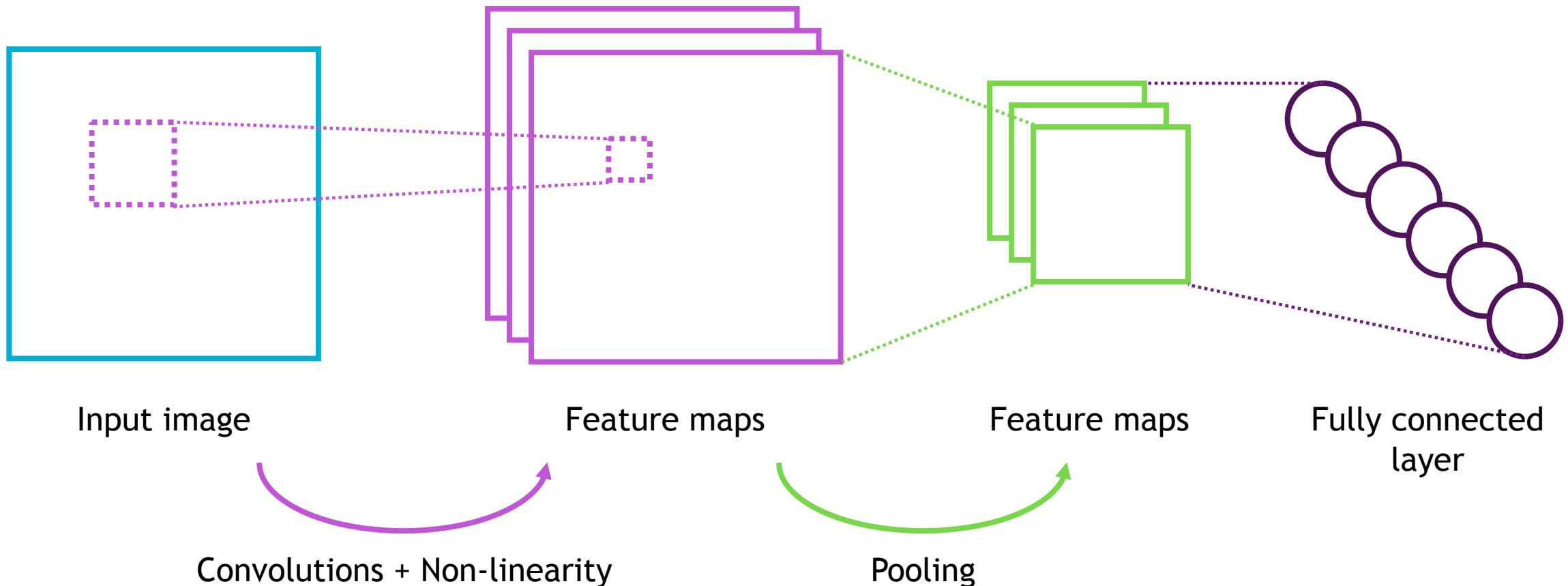
Horizontal edge detection

Using spatial features

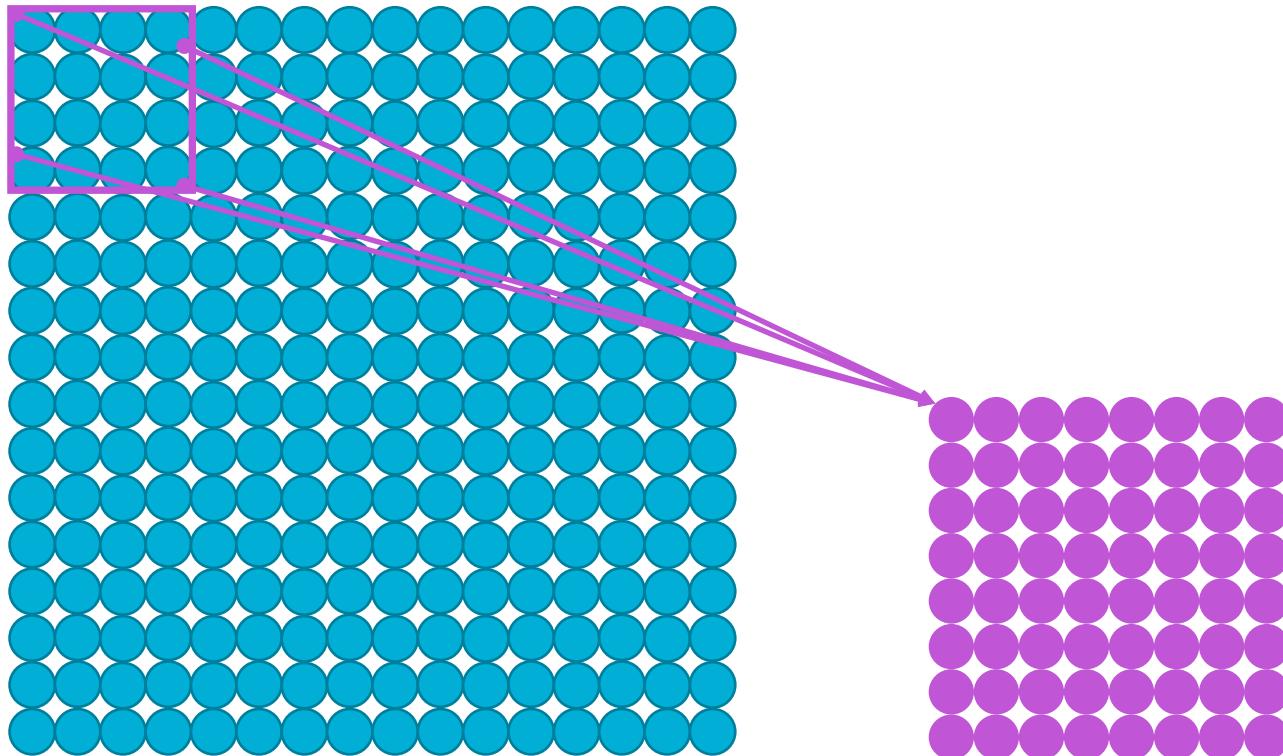


- Apply a set of weights - a filter - to extract **local features**
- Use **multiple filters** to extract different features

CNNs for classification



Convolutional layer



Neuron (p, q) in hidden layer

Filter size 4×4

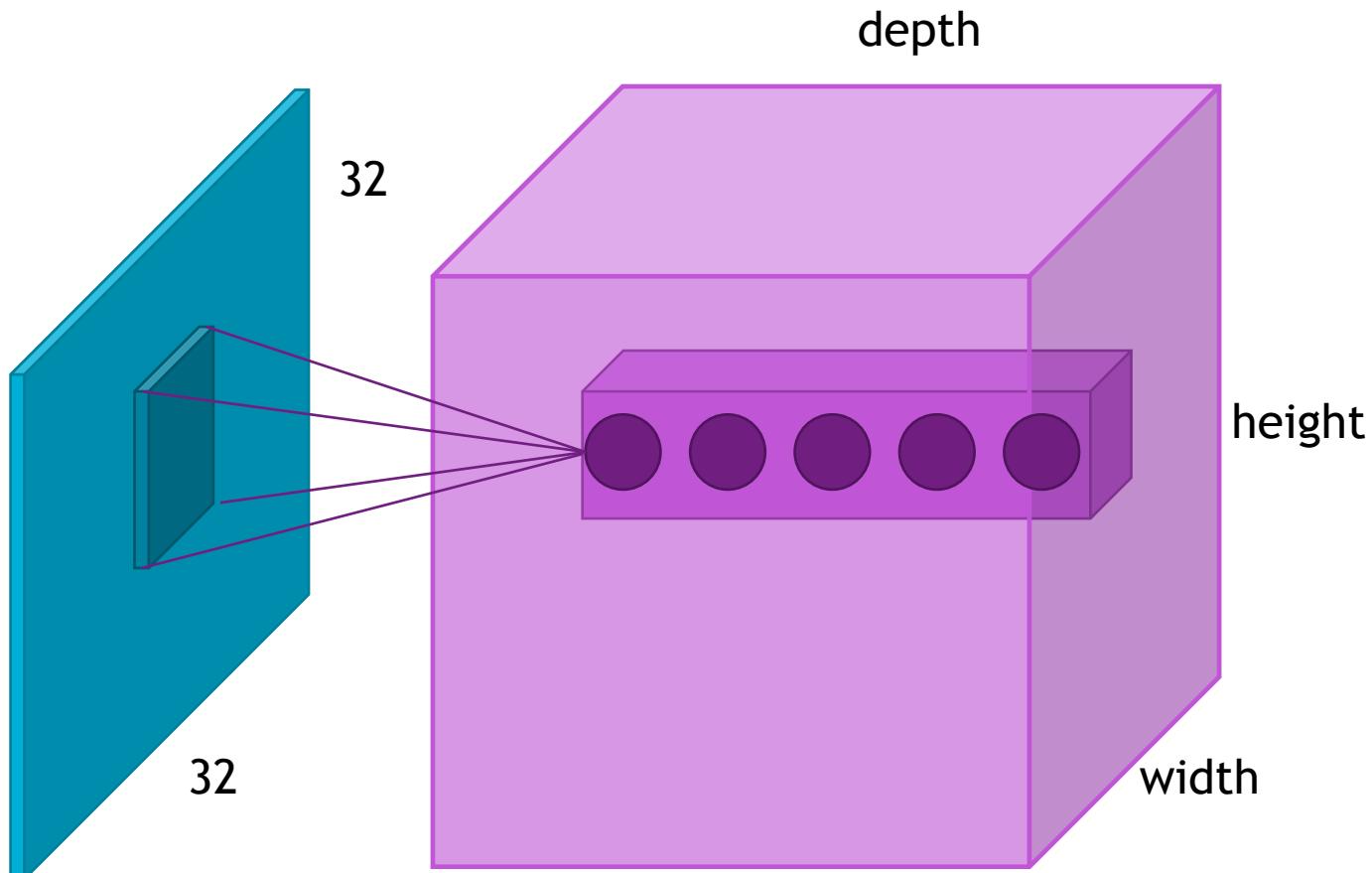
Weights $w_{i,j}$

$$h \left(\sum_{i=1}^4 \sum_{j=1}^4 w_{i,j} x_{i+p, j+q} + b \right)$$

For a neuron in hidden layer:

- Take inputs from patch
- Compute weighted sum
- Apply bias
- Activate with non-linear function

Spatial arrangement of output volume



1

Layer Dimensions:

$$h \times w \times d$$

h & w = spatial dimensions
 d = number of filters

Stride:

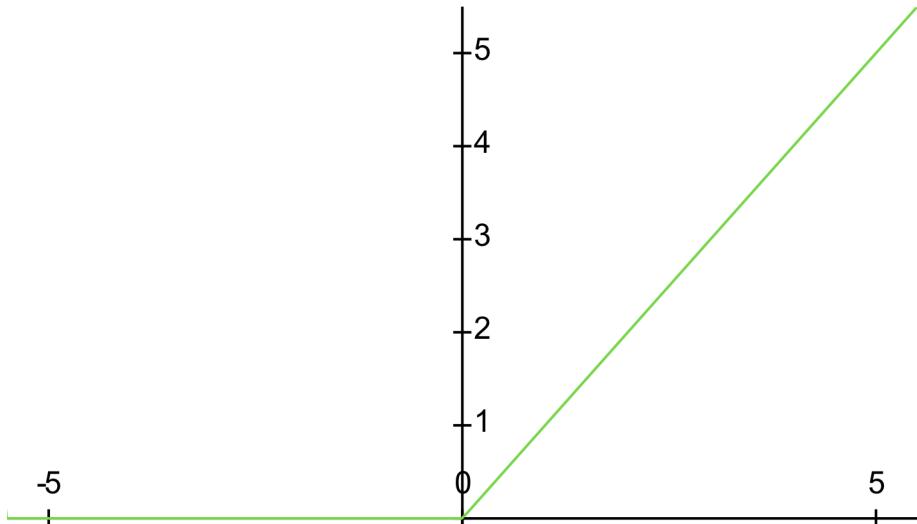
Filter step size

Receptive Field:

Locations in input image that a node is connected to

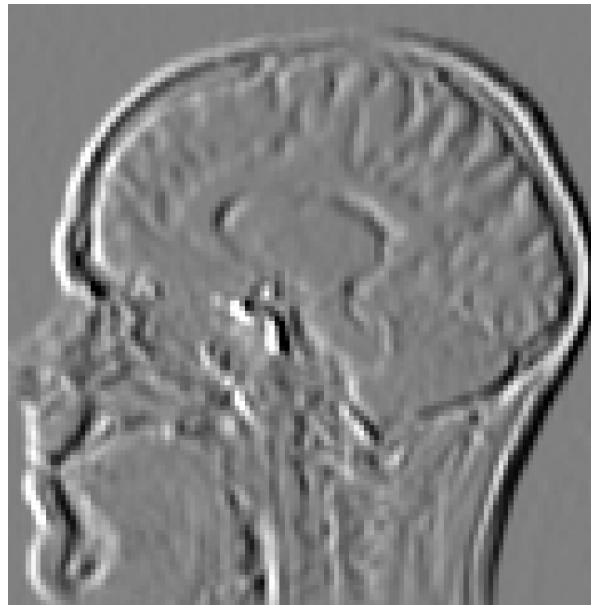
Introducing non-linearity

Rectified linear unit (ReLU)

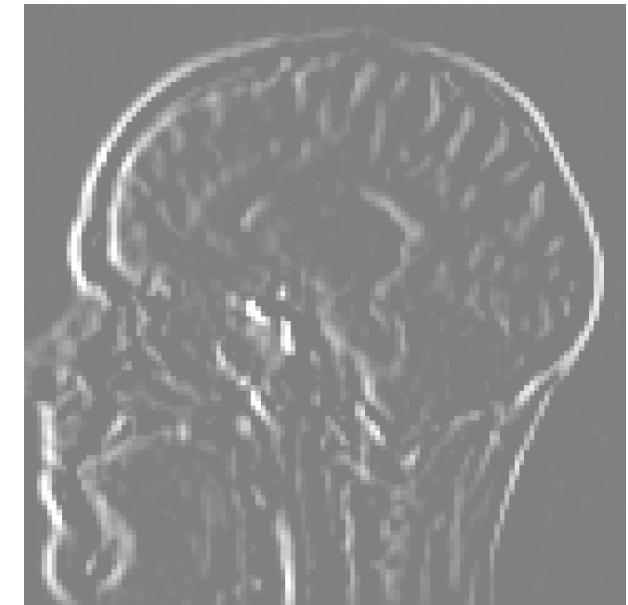


$$h(z) = \max(0, z)$$

Input feature map



Rectified feature map



ReLU

Black: negative values - White: positive values

Pooling

- Reduce dimensionality while preserving spatial invariance

Input feature map

1	1	8	3
4	7	1	9
5	3	1	4
2	3	6	0

Max pooling with
 2×2 filter and stride 2



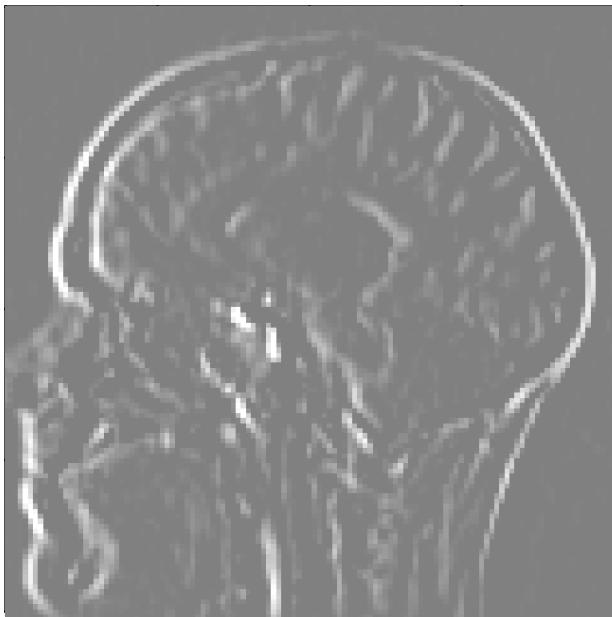
Pooled feature map

7	9
5	6

Pooling

- Reduce dimensionality while preserving spatial invariance

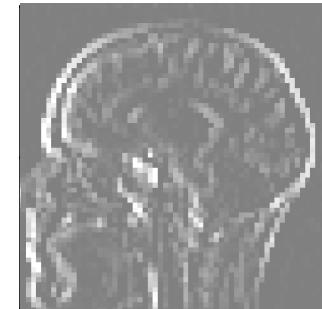
Input feature map



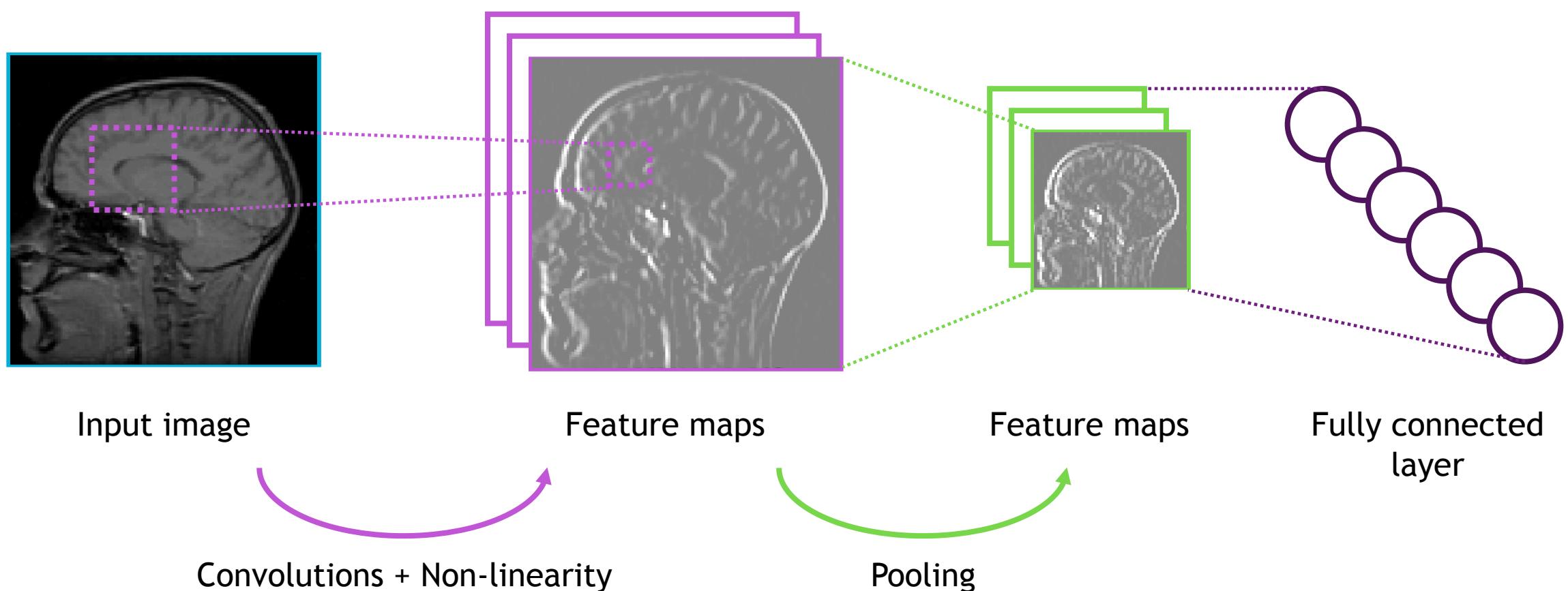
Max pooling with
 2×2 filter and stride 2



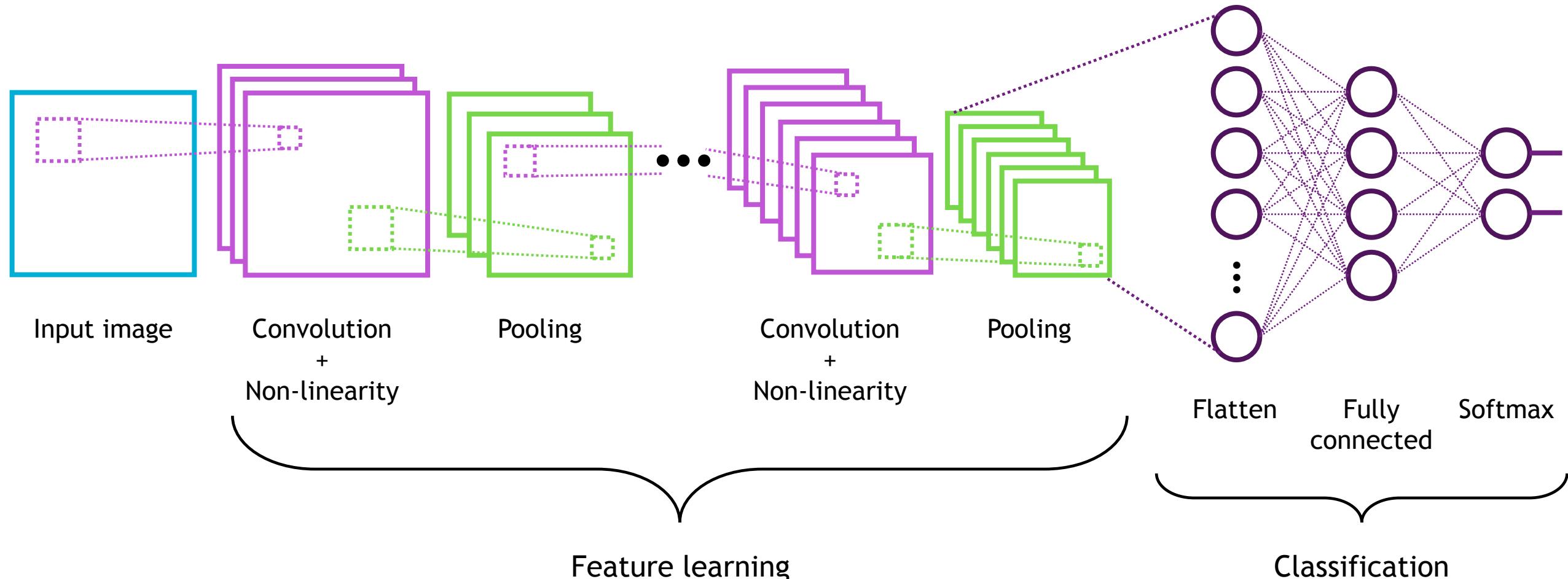
Pooled feature map



CNNs for classification

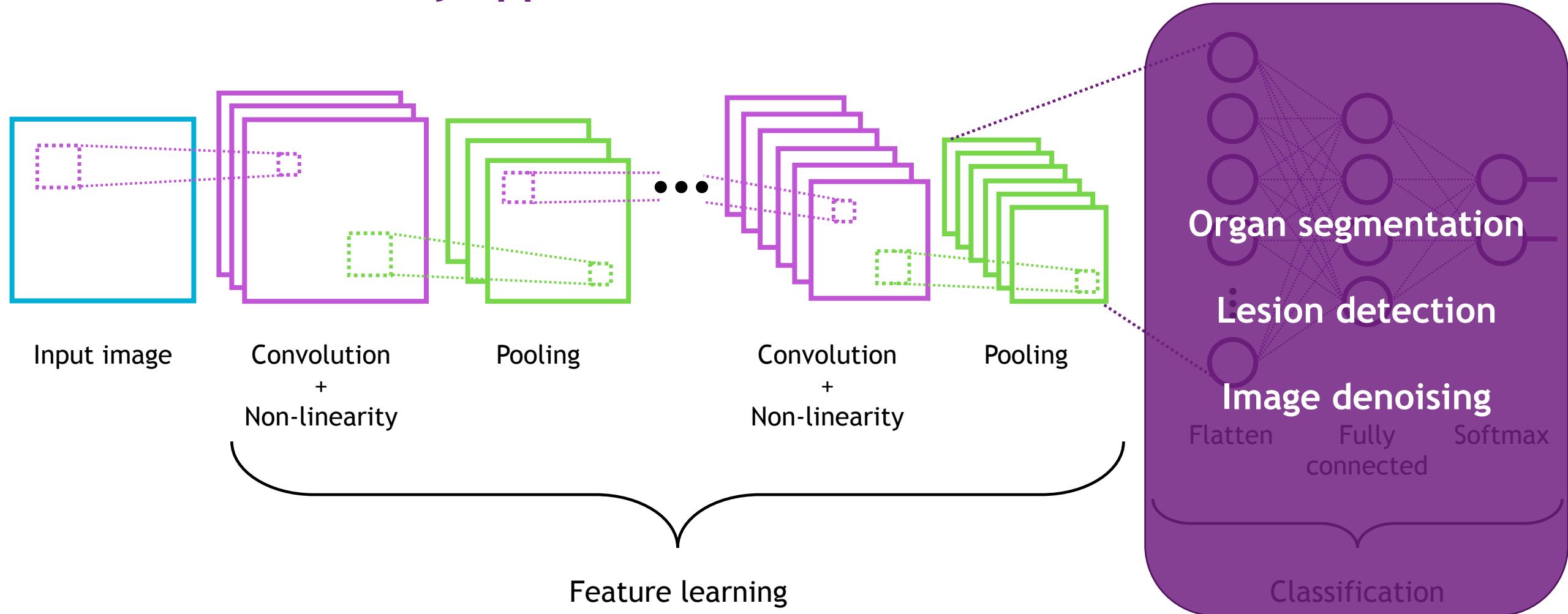


CNNs for classification



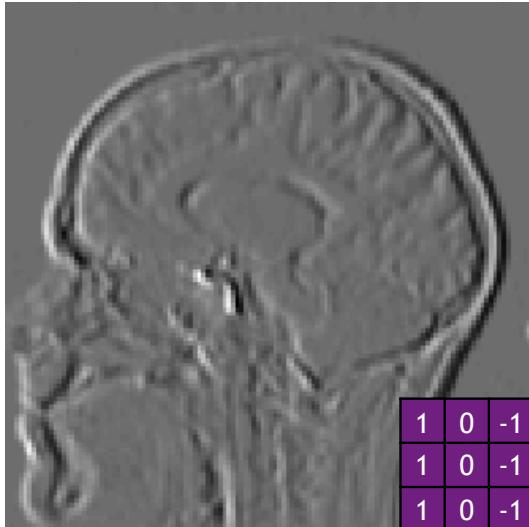
Convolutional neural networks

CNNs for many applications



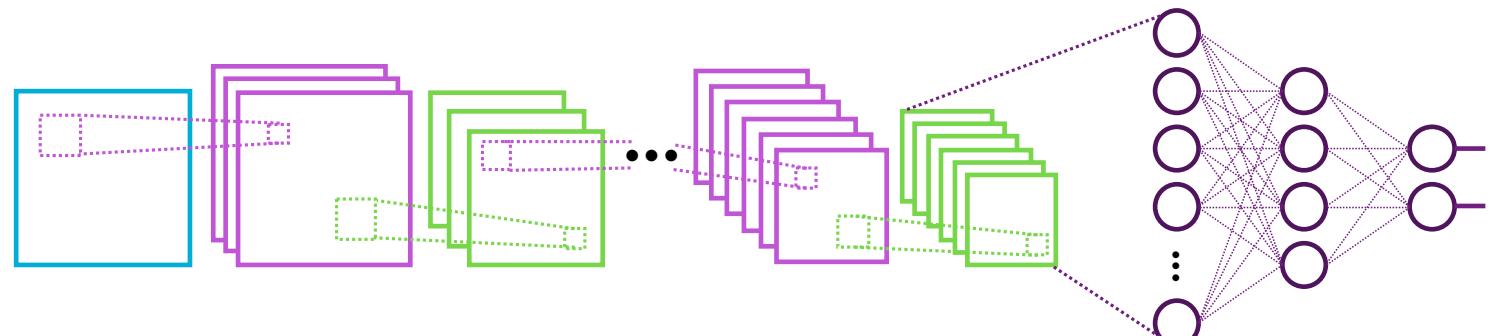
Images

- Representing images
- Convolutions for feature extraction



CNNs

- Convolution → non-linearity → pooling
- Stacking layers

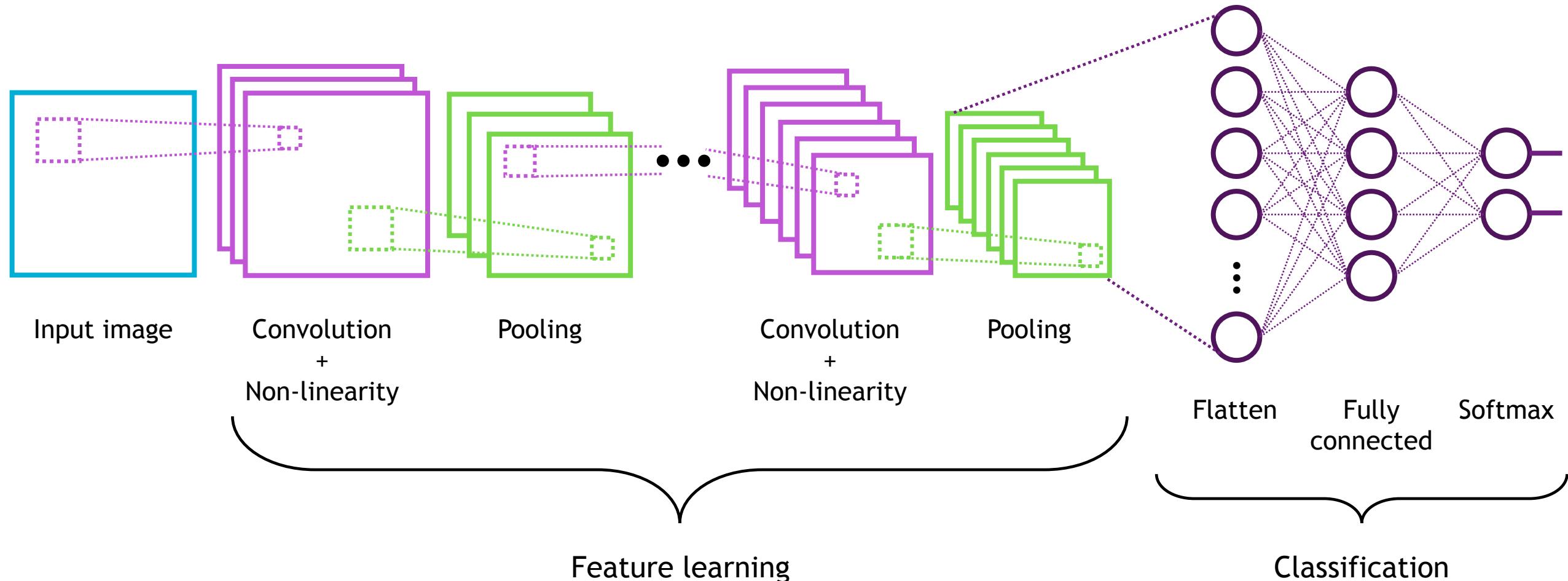


Applications

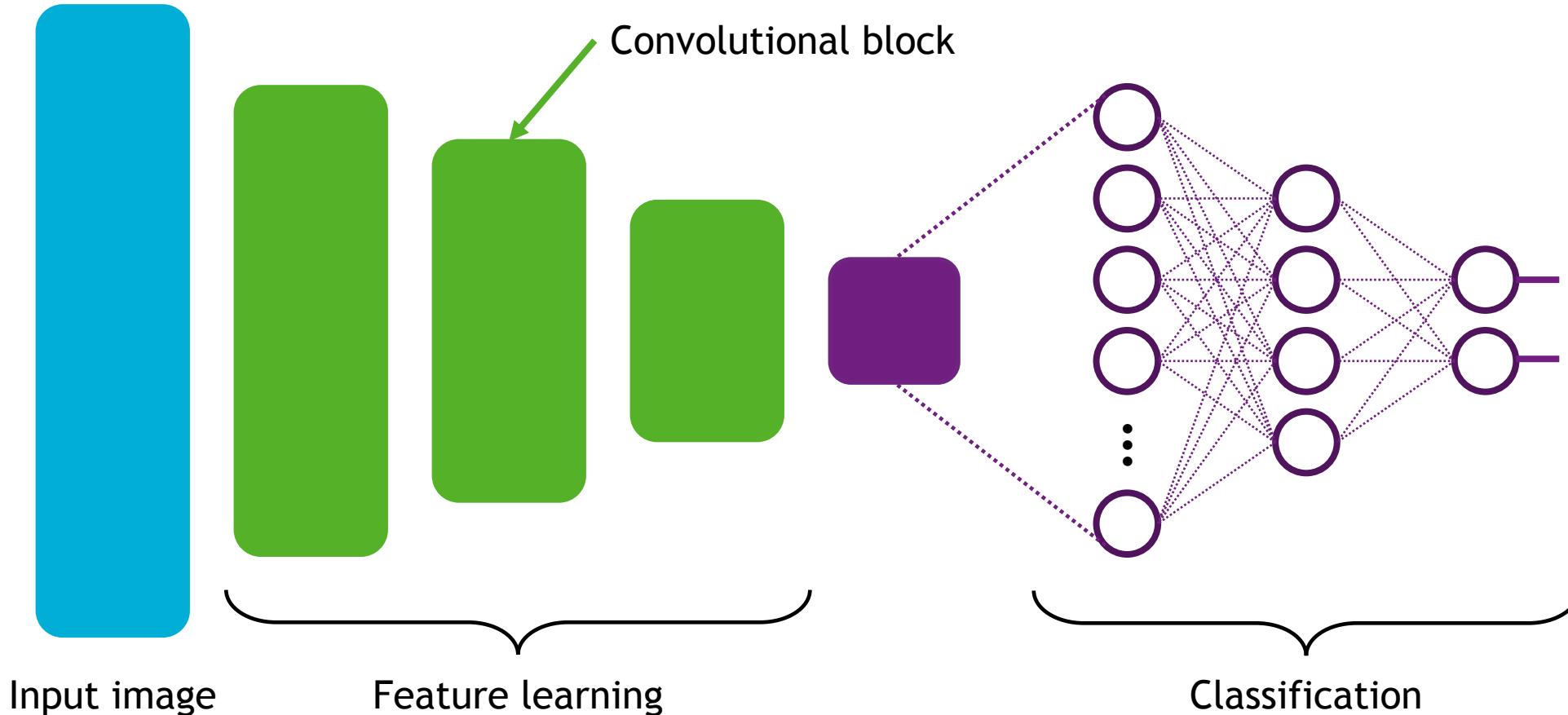
- Classification
- Segmentation
- Detection

Generative Deep Learning

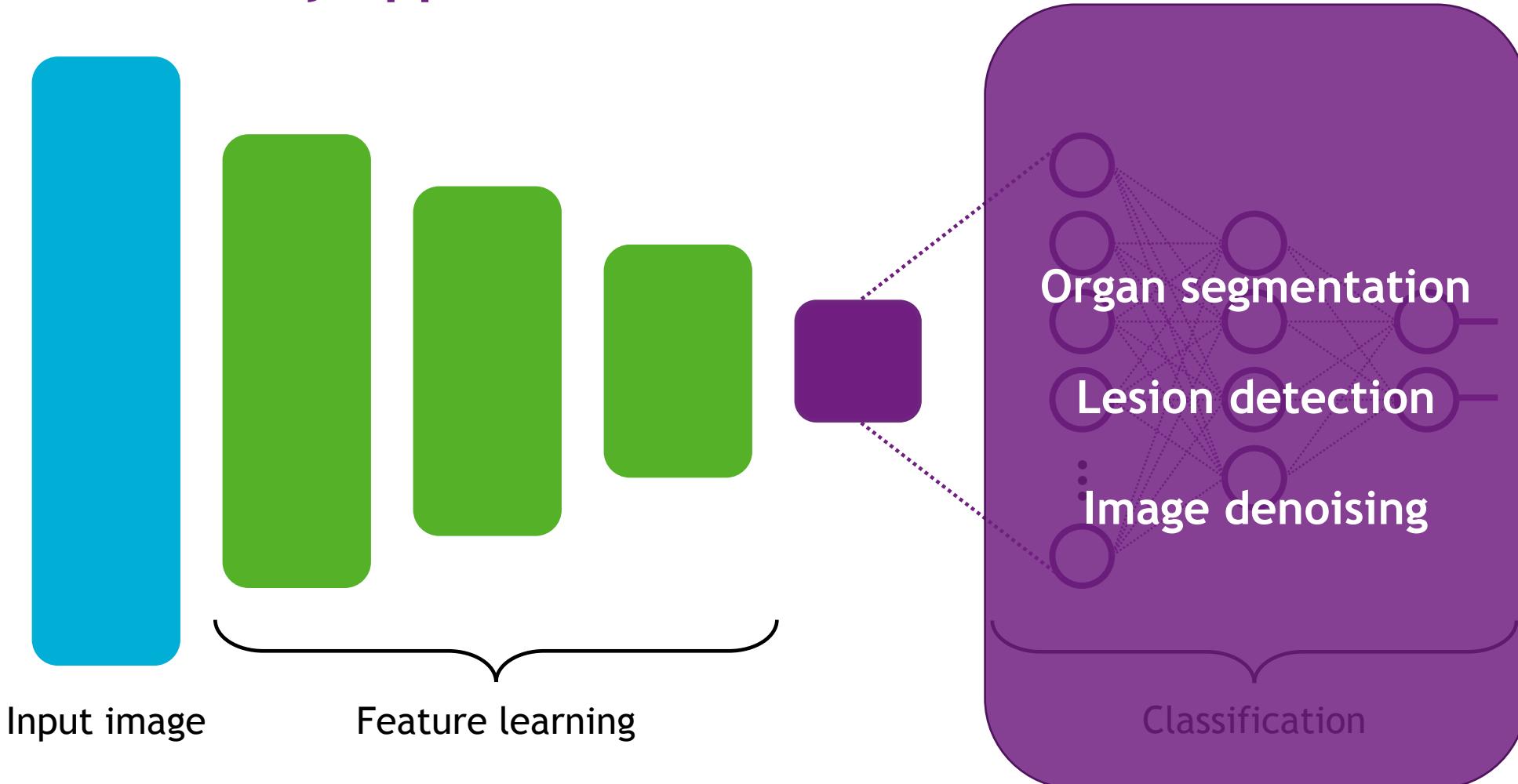
CNNs for classification



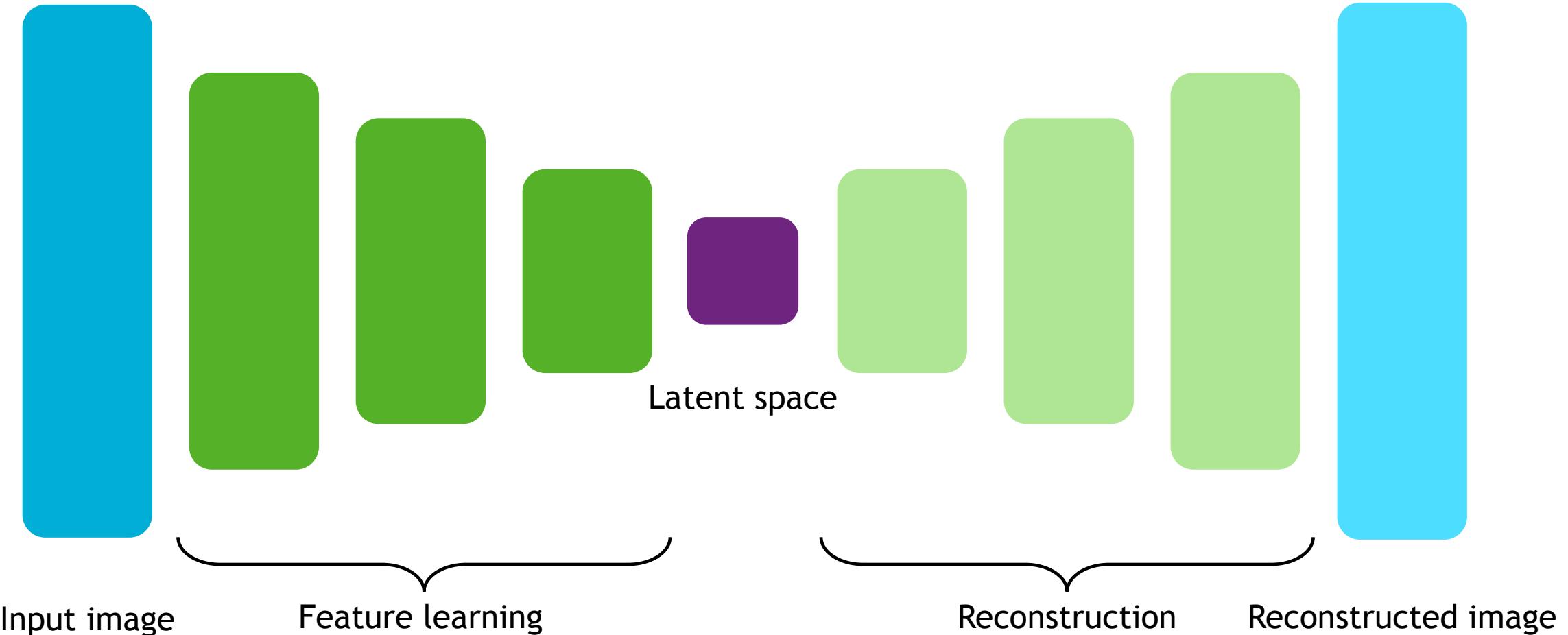
CNNs for classification



CNNs for many applications



CNNs for image generation



Latent variable

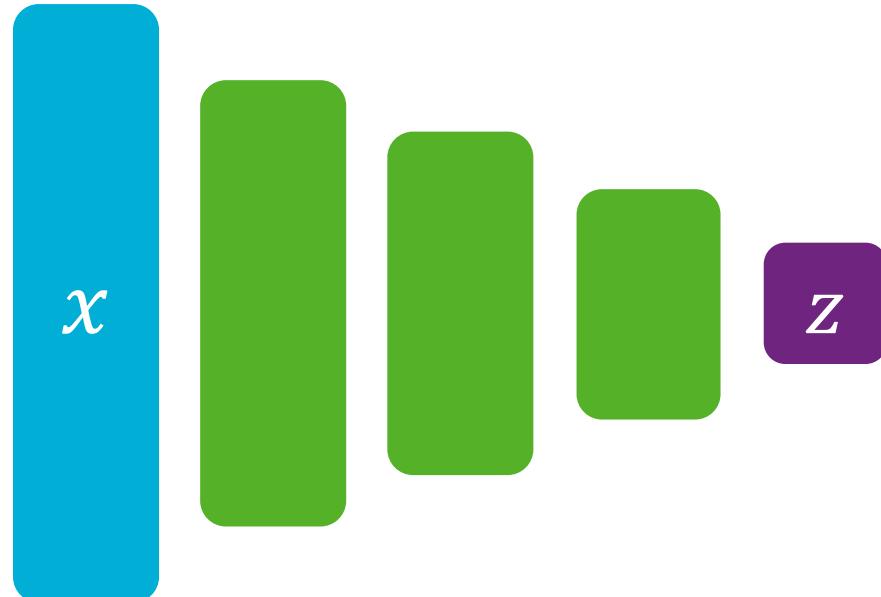
Observed variable



Latent variable



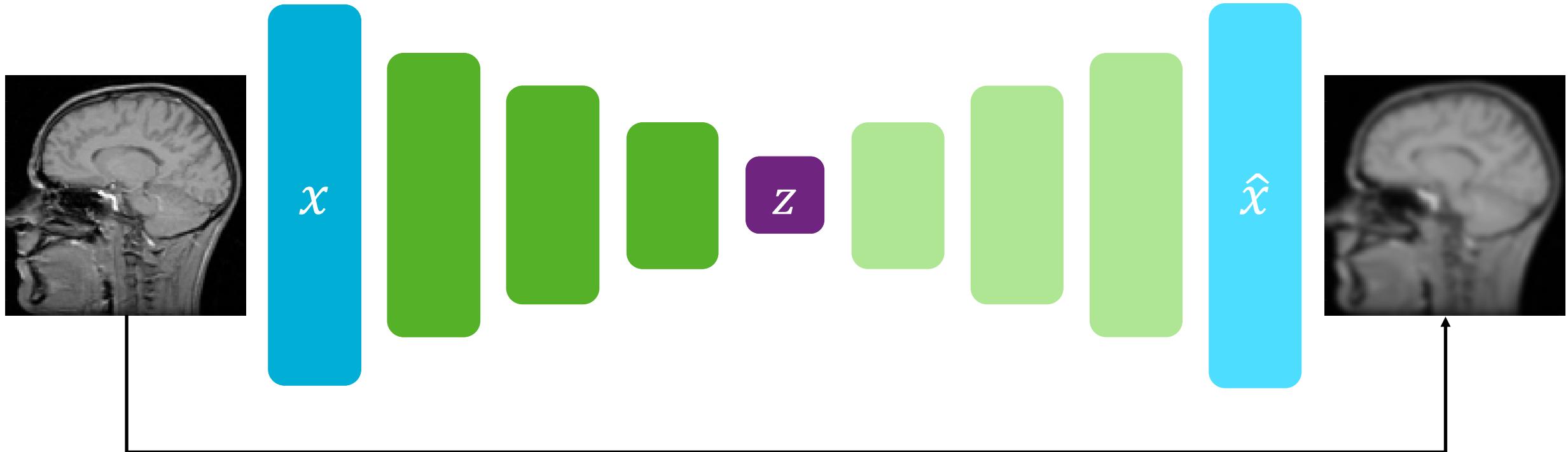
Encoder



Input image
=
observed data

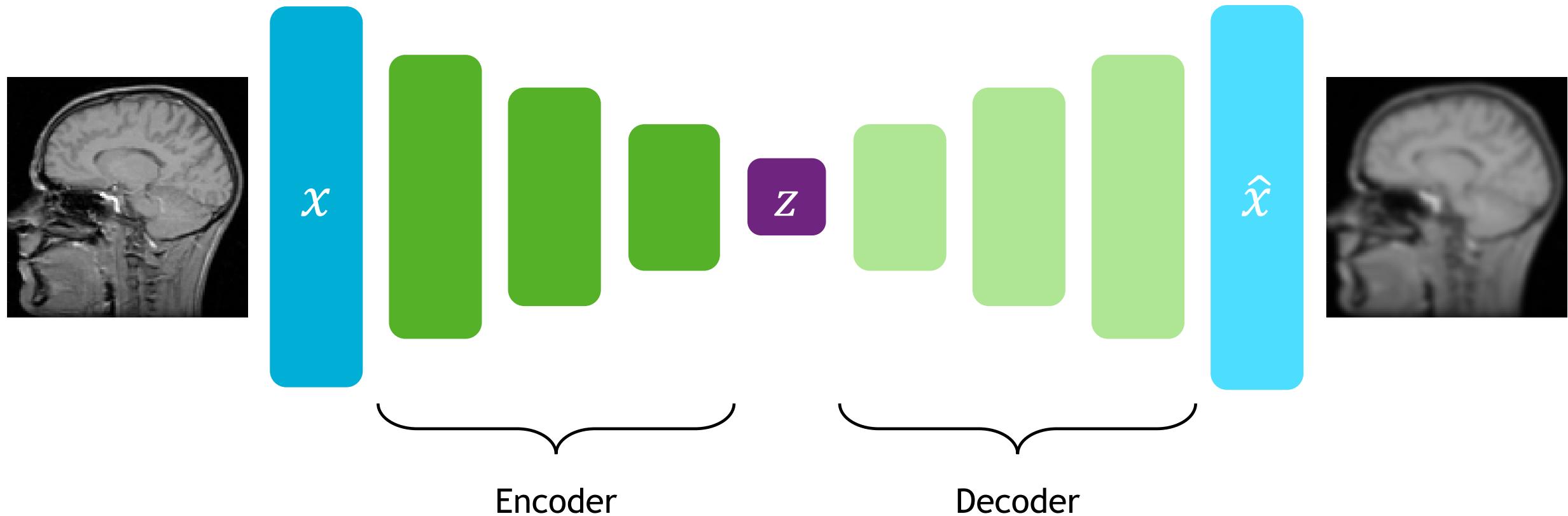
Latent space
=
low dimensional representation
of the observed data

Training autoencoders

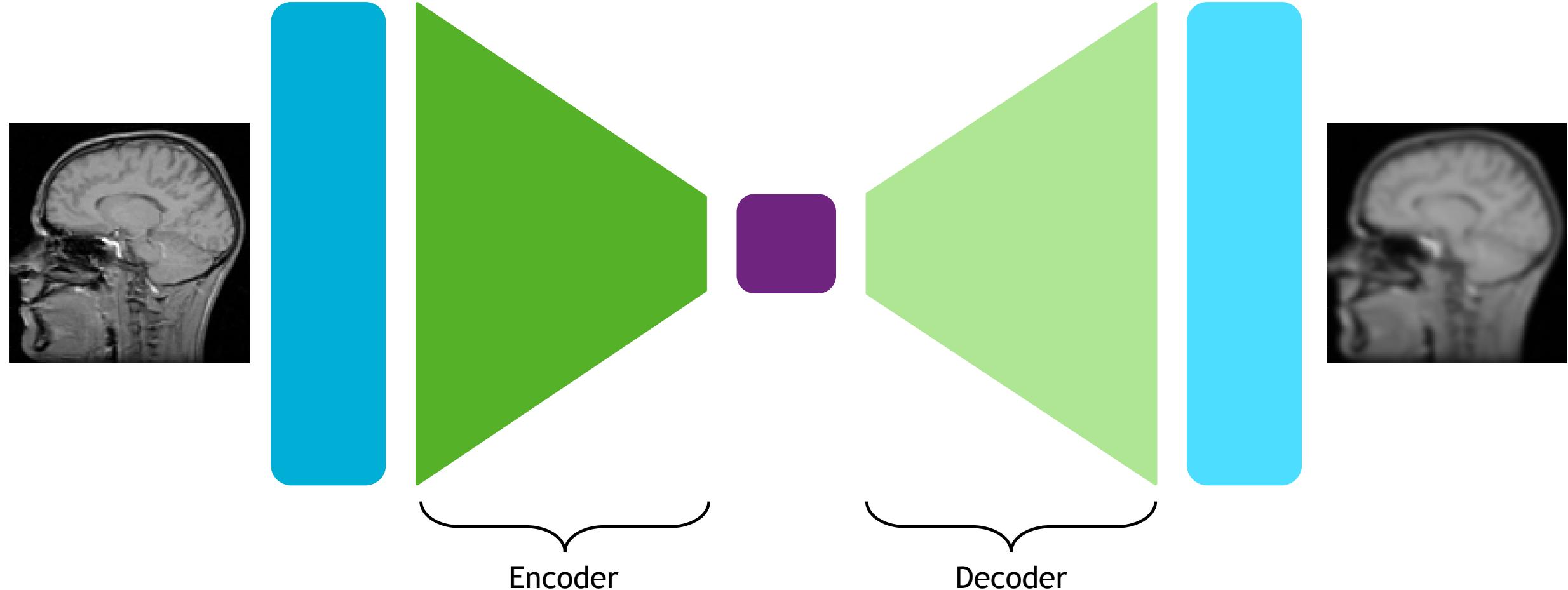


$$\mathcal{L}(x, \hat{x}) = \|x - \hat{x}\|^2$$

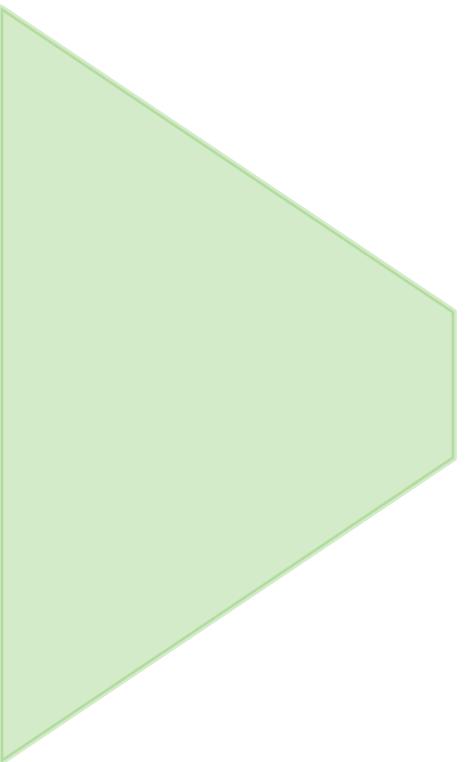
Autoencoders



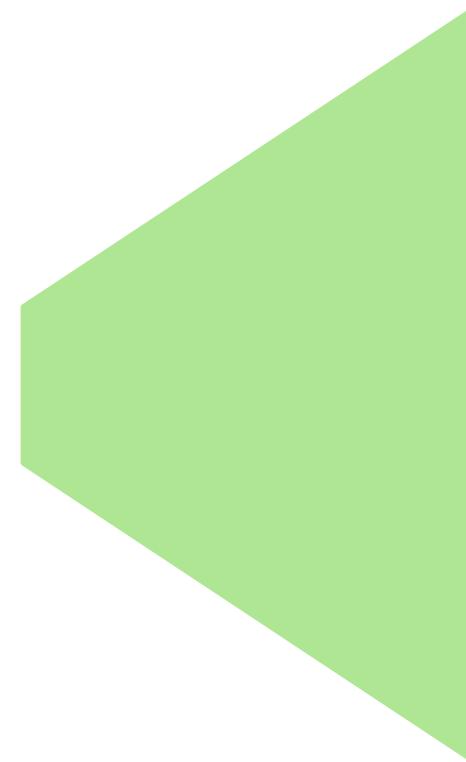
Autoencoders



Generating images from scratch

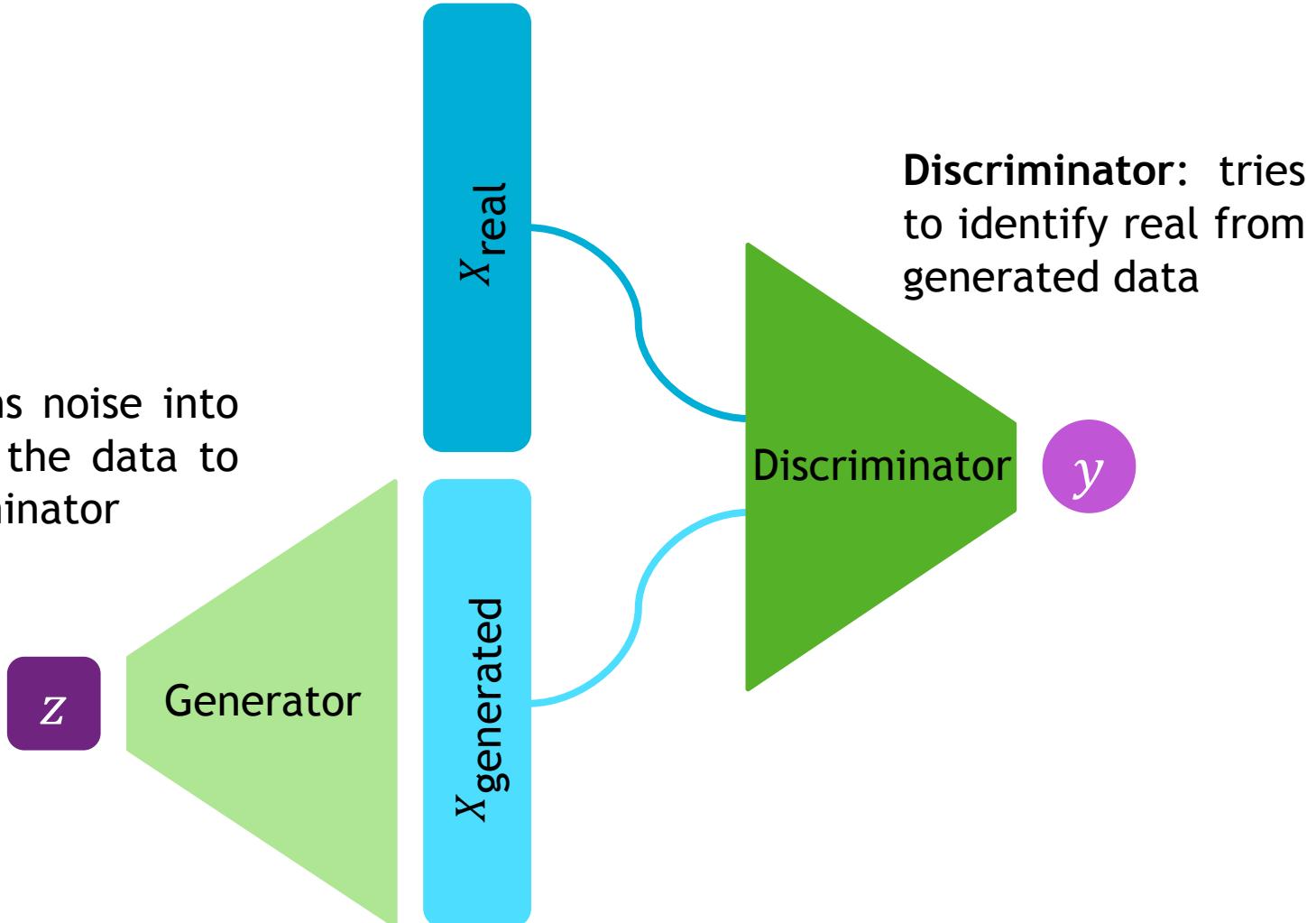


Random
noise



Competing networks

Generator: turns noise into an imitation of the data to trick the discriminator



Generating new images

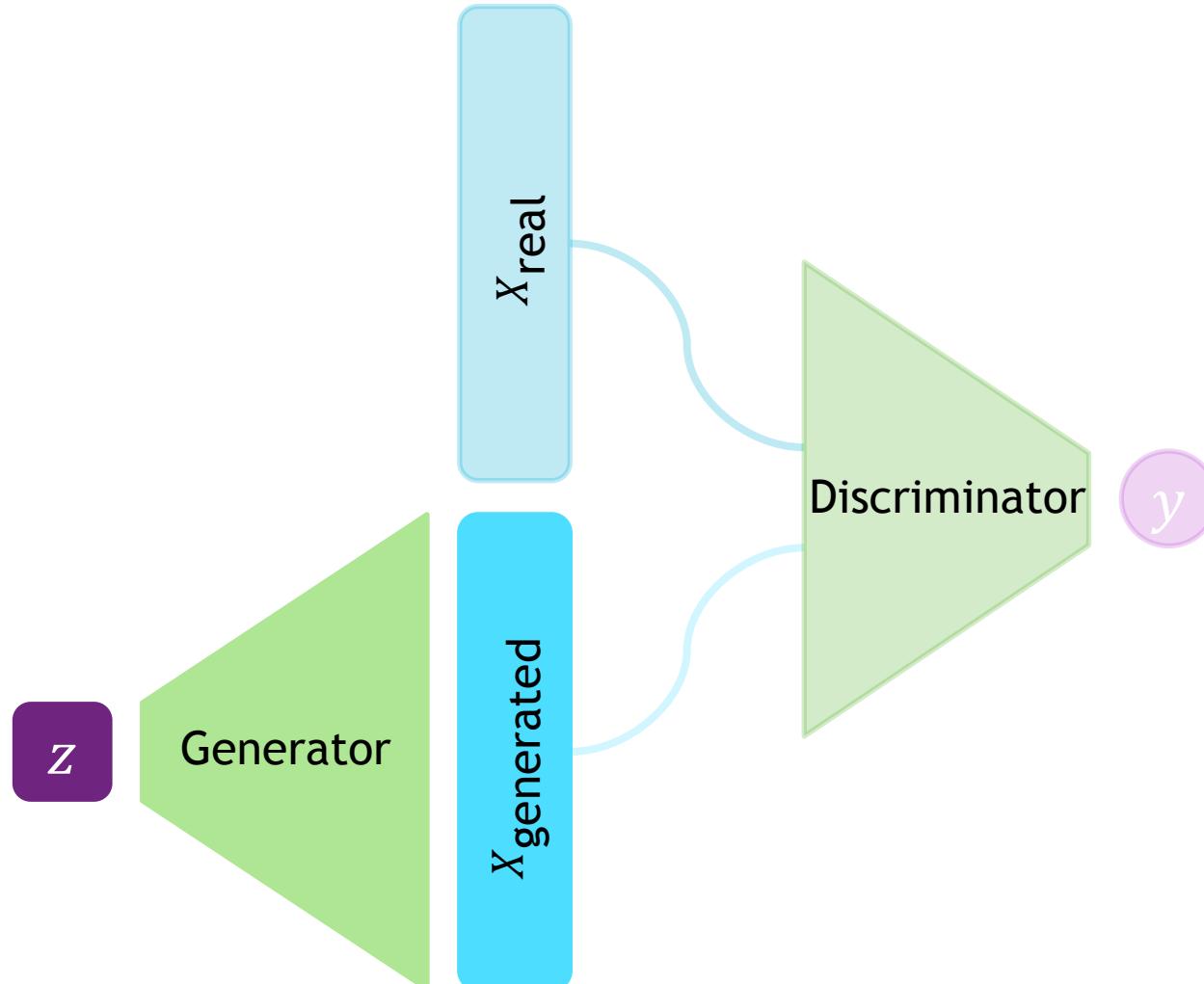


Image translation with conditional GANs

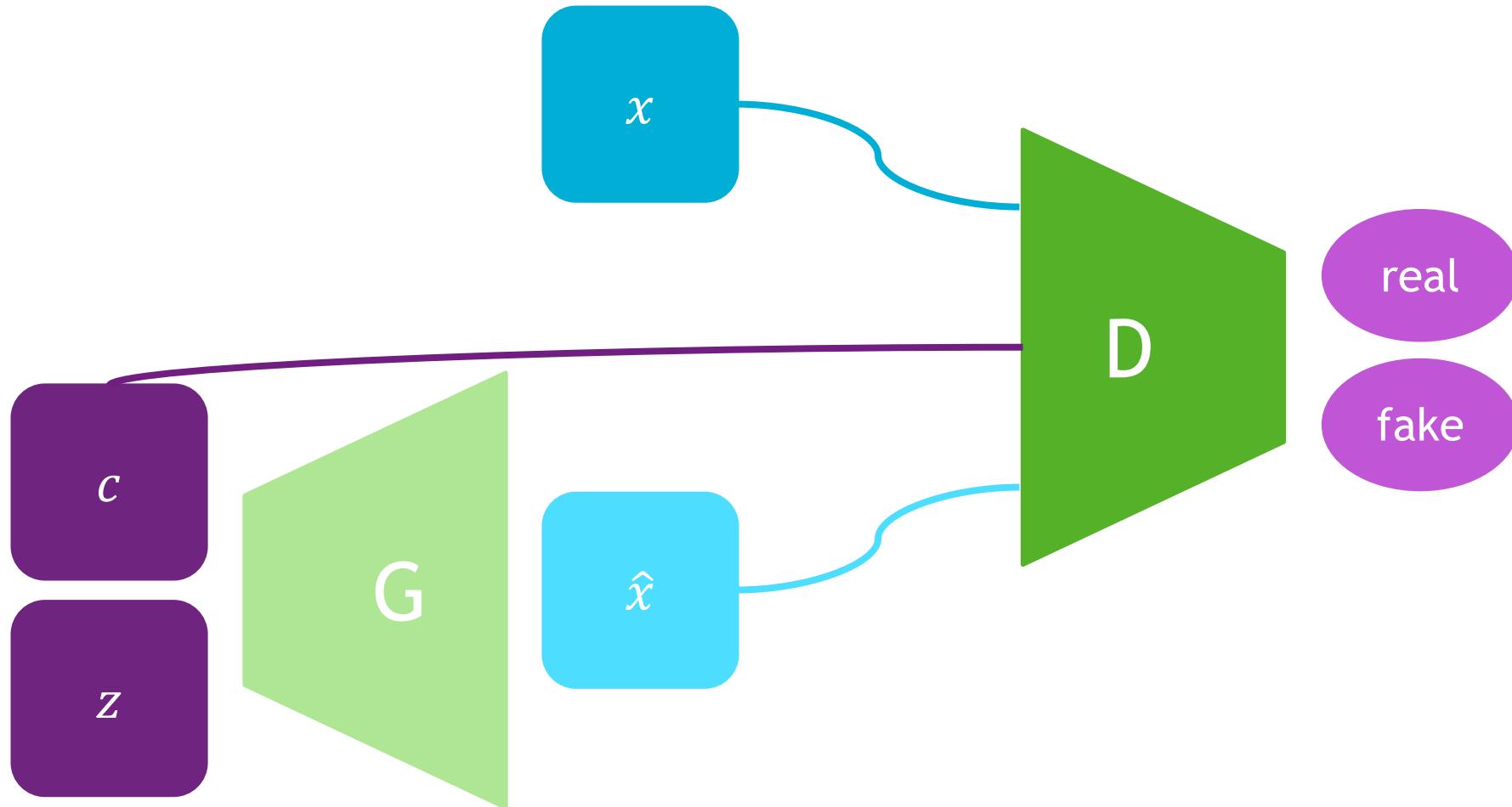


Image translation with conditional GANs

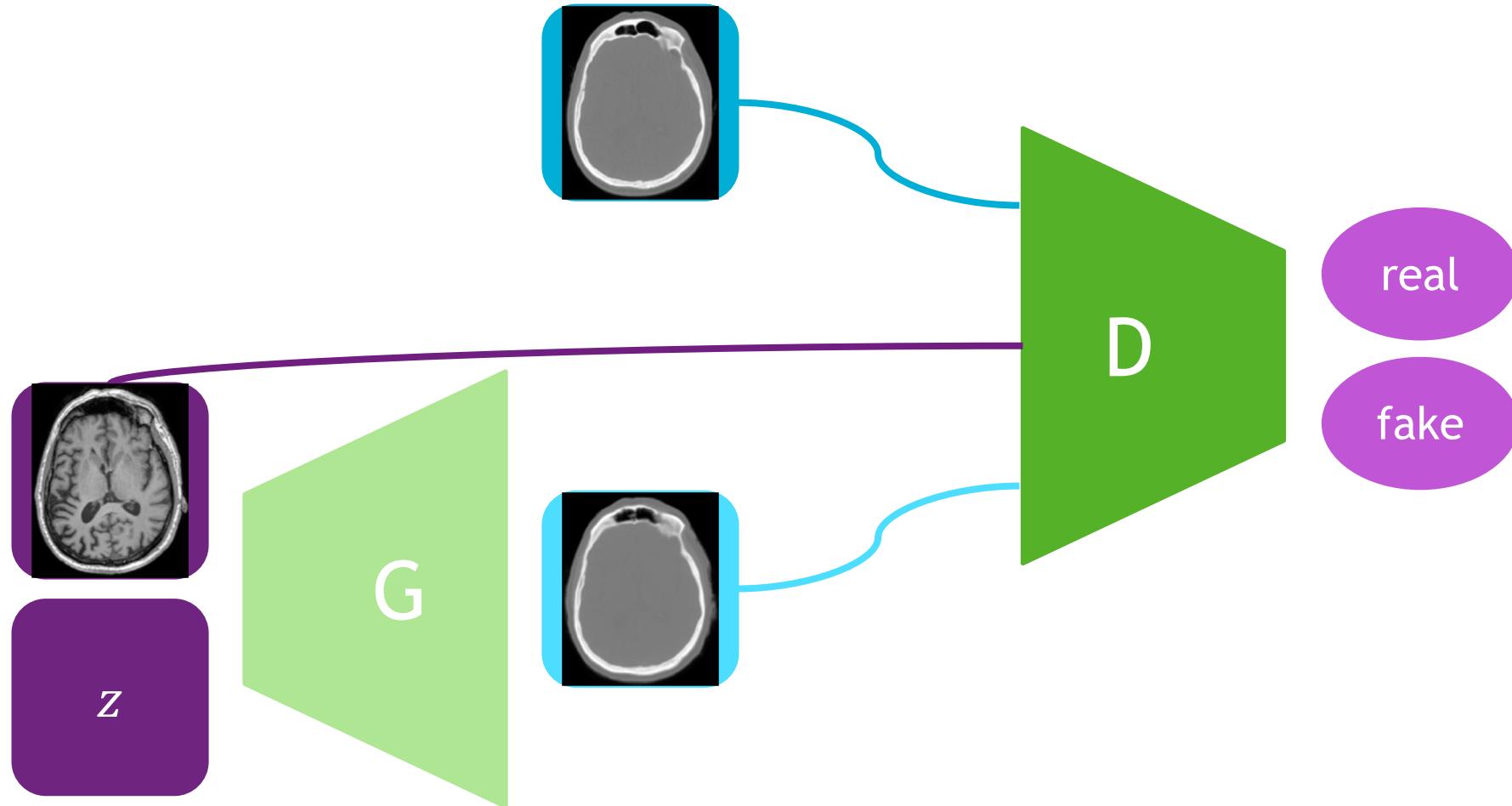
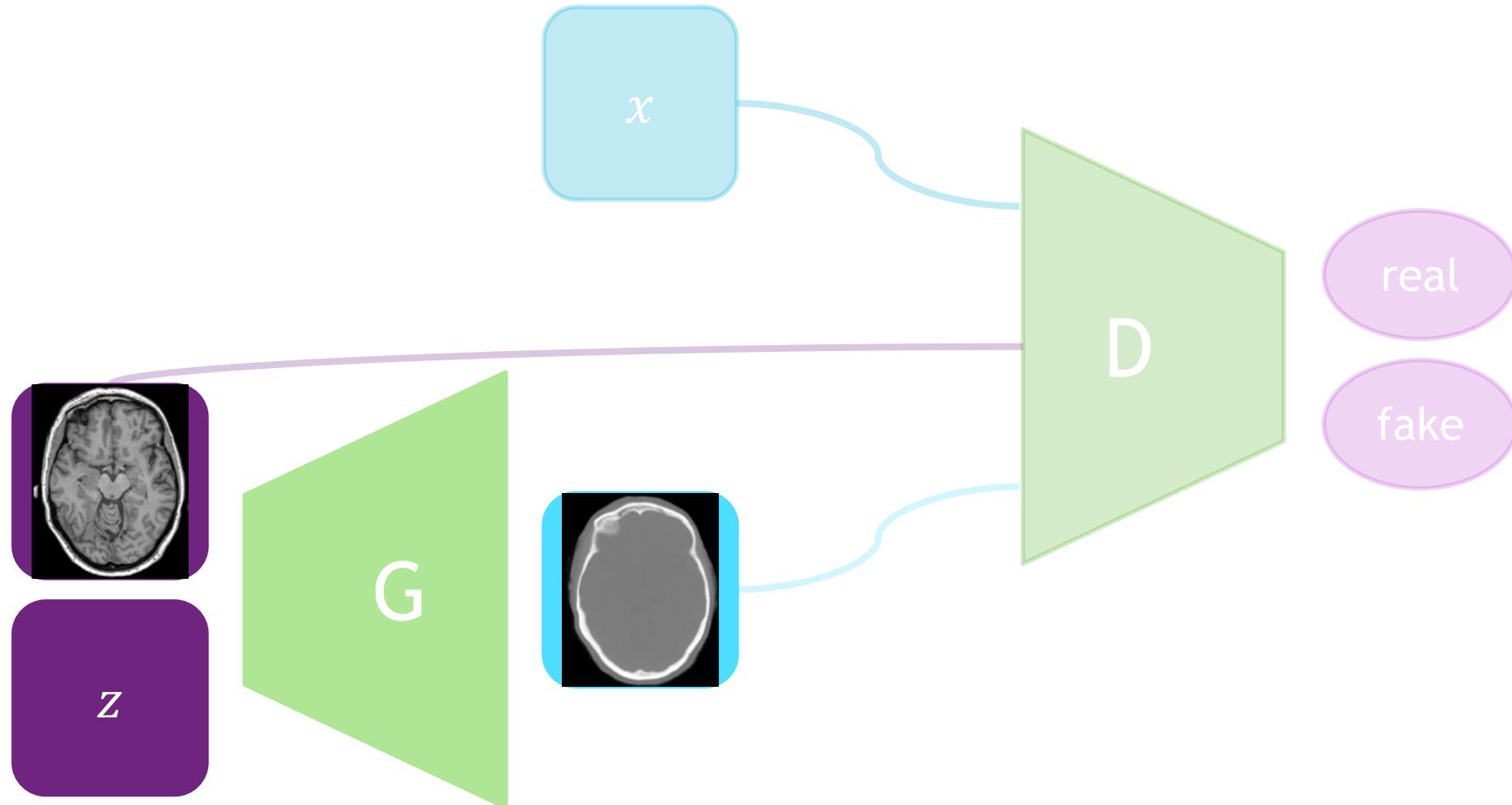
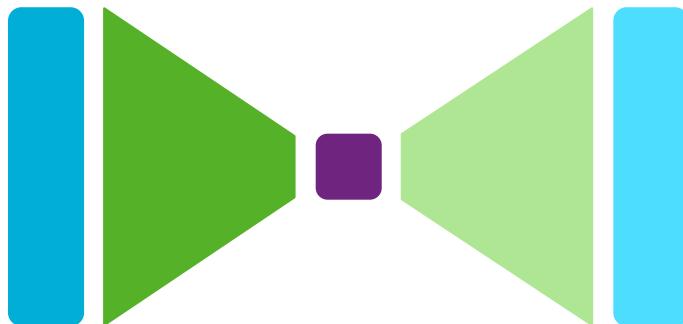


Image translation with conditional GANs



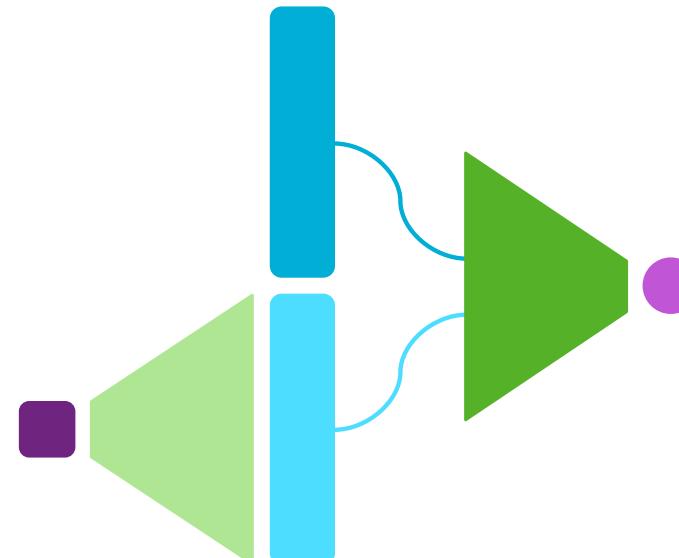
Autoencoders

- Learn low dimensional latent space



GANs

- Competing generator and discriminator networks



Conditional GANs

- For image translation

