Neural Networks I

Supervised learning in practice

Preprocessing
Explore & prepare data

Data Visualization and Exploration

Identify patterns that can be leveraged for learning

Data Cleaning

- Missing data
- Noisy data
- Erroneous data

Scaling (Standardization)

Prepare data for use in scale-dependent algorithms.

Feature Extraction

Dimensionality reduction eliminates redundant information

Model training

1 Supervised Learning Models: Linear models and KNN
(enough to get started using supervised learning)

5 Other algorithms and concepts:

- Generative vs discriminative models
- Parametric vs nonparametric models
- Model ensembles
- **Feature/representation learning (neural networks, deep learning)**

4 How to control model overfit: regularization strategies for model refinement

Iteratively fine tune the model

Performance evaluation

Make a prediction on validation data

2 Evaluating model performance and comparing models

Precision, Recall, F_1,

3 How to make decisions using models

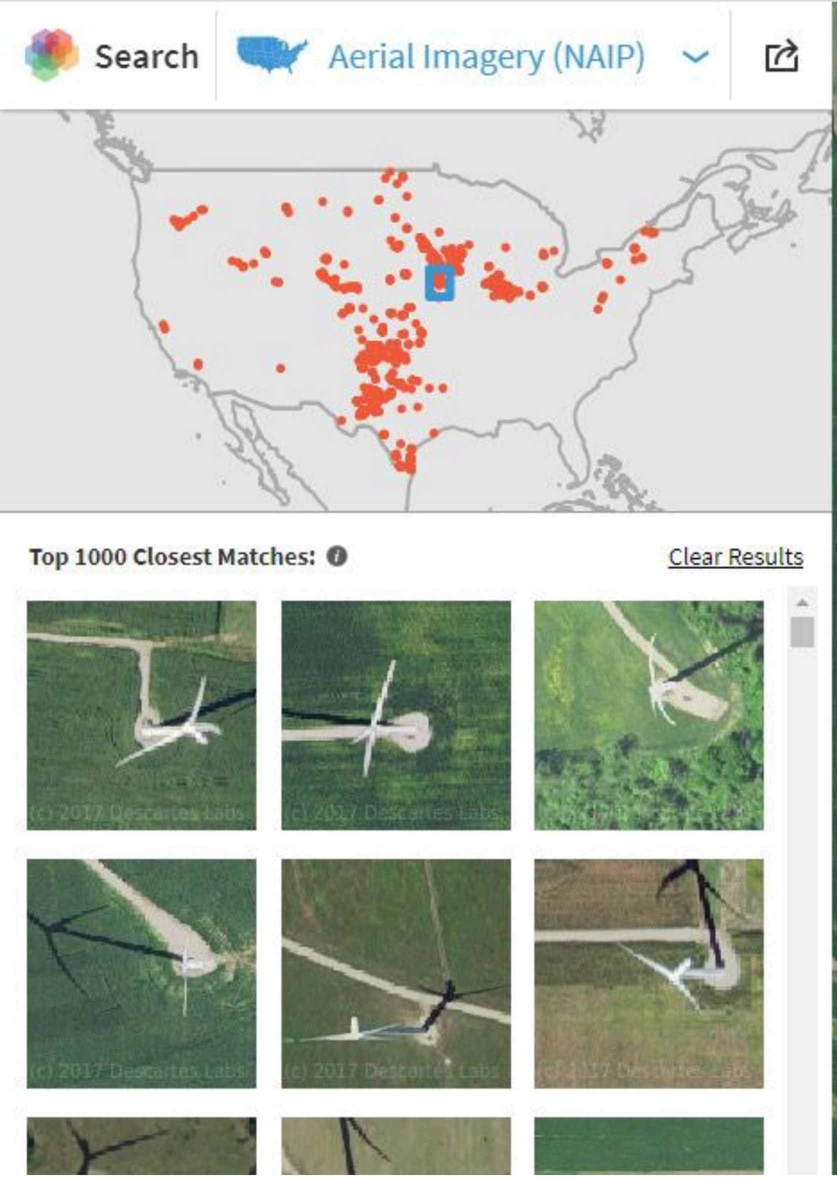
Regression
MSE, explained variance, R^2

Neural networks are not appropriate for every problem

- Small datasets
- Tabular data
- Cases when model interpretability is paramount

What's the hype around neural networks?

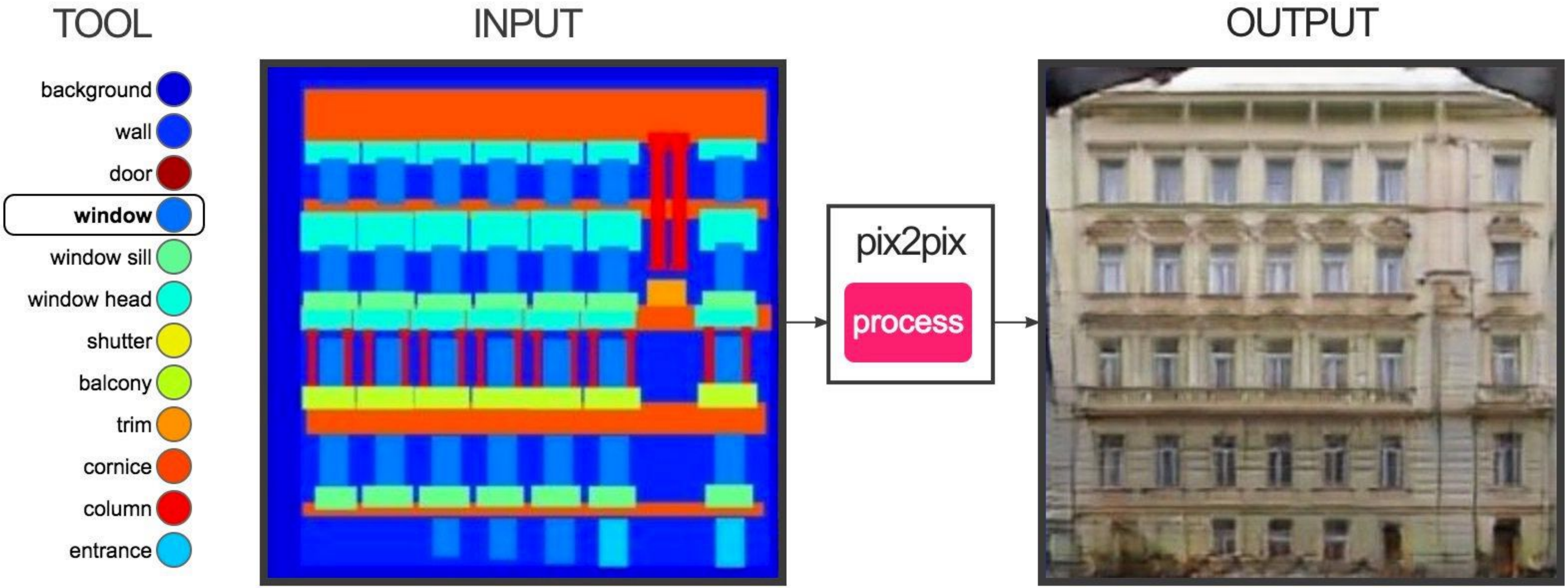
Character/handwriting recognition
Self-driving cars
Natural language processing and translation
Speech recognition
Medical devices, diagnosis, and treatment
Materials development
Automated financial trading systems
Industrial automation
Computer vision applications…



Geovisual Search

https://search.descarteslabs.com/

Image-to-image translation



Isola, Phillip, et al. "Image-to-image translation with conditional adversarial networks." arXiv preprint (2017).

Image-to-image translation

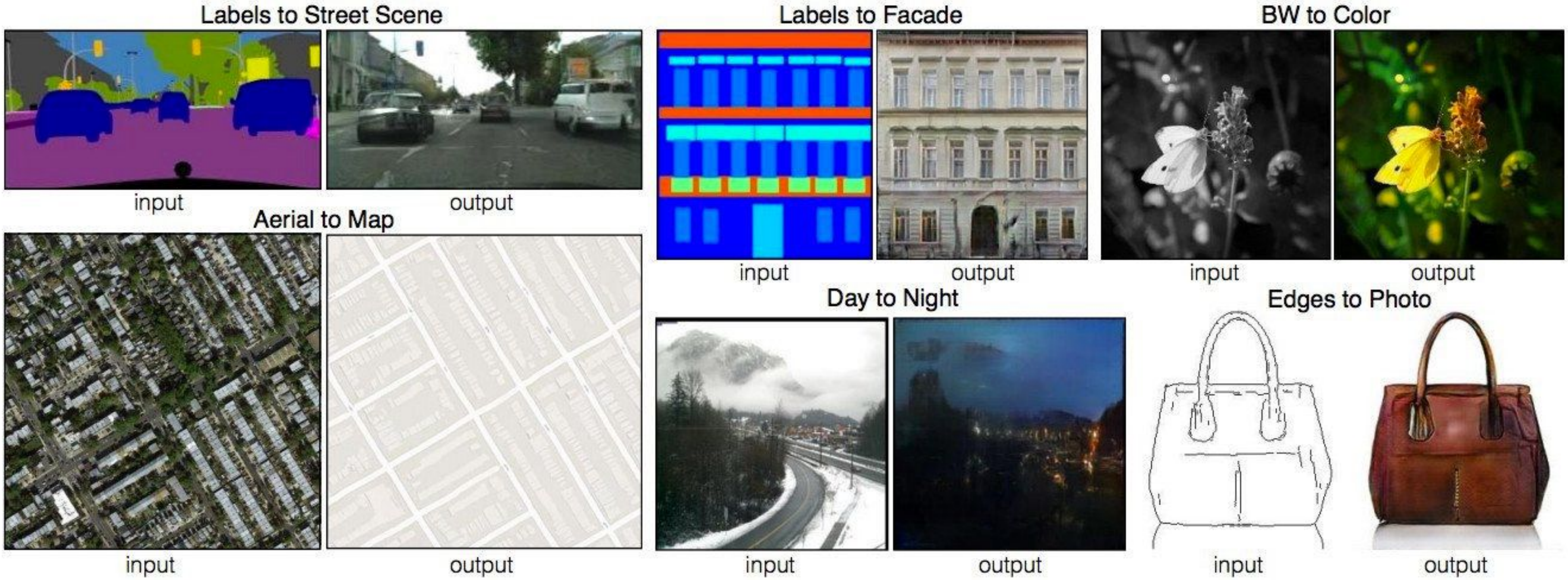


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Image-to-image translation

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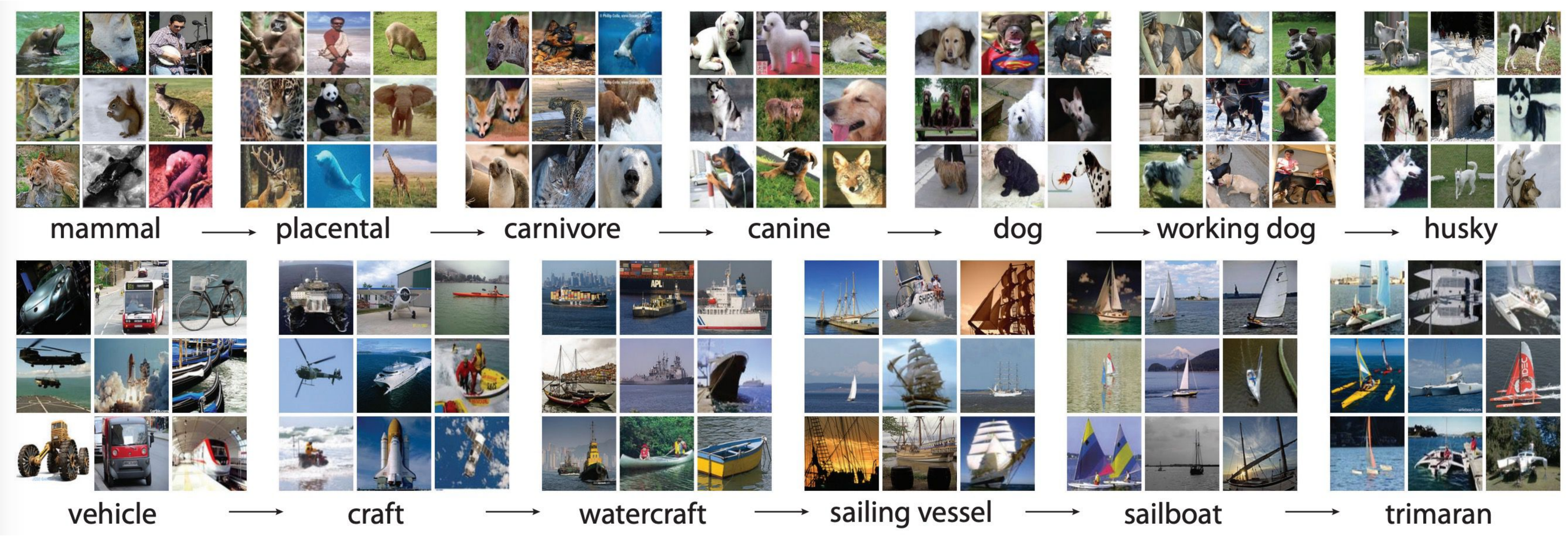
Image Style Transfer

Dumoulin, Vincent, Jonathon Shlens, and Manjunath Kudlur. "A learned representation for artistic style." CoRR, abs/1610.07629 2.4 (2016): 5.

ImageNet Competition

- Image classification challenge
- 14,197,122 annotated images
- 1,000 classes

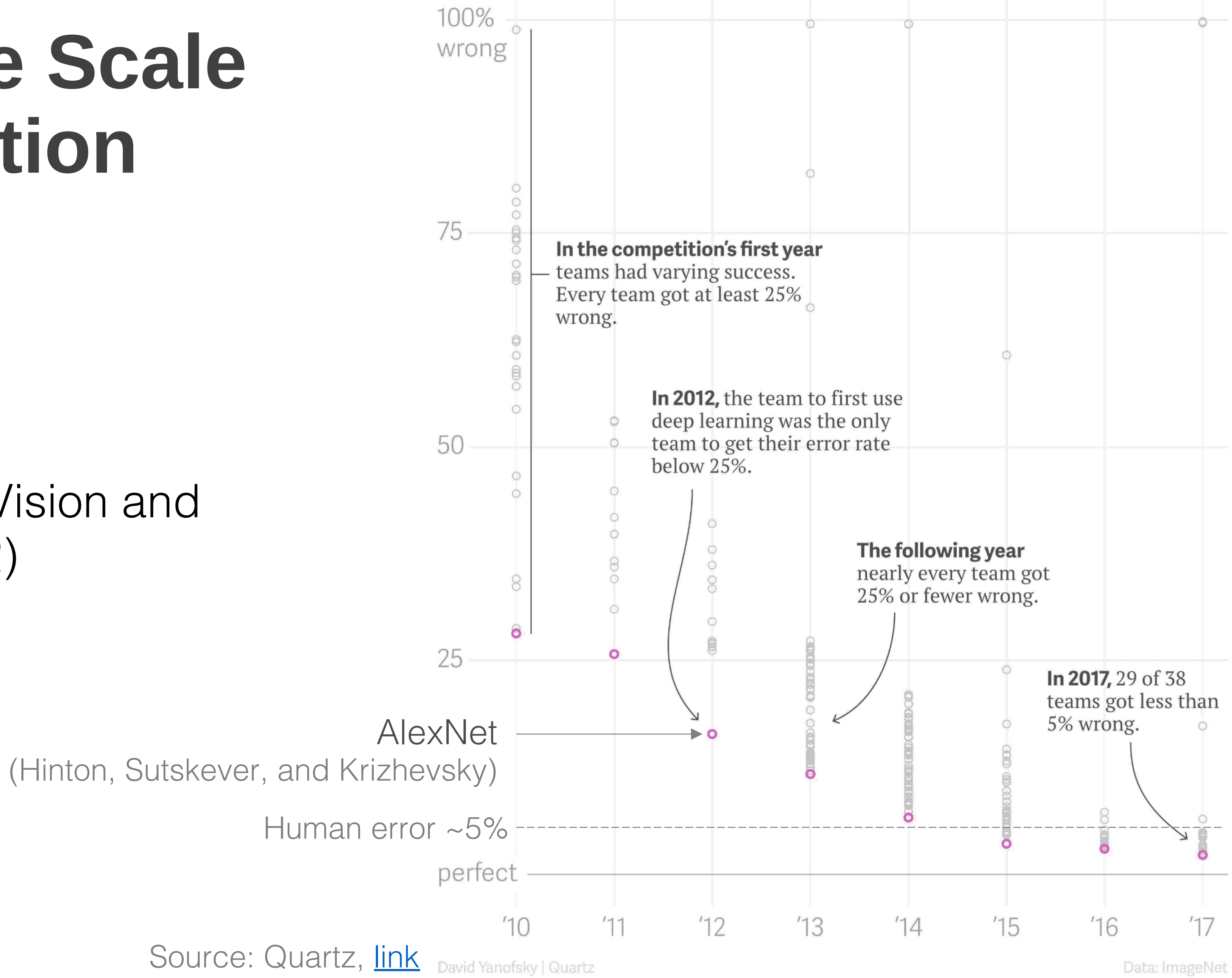


Deng, J., Dong, W., Socher, R., Li, L.J., Li, K. and Fei-Fei, L., 2009, June. Imagenet: A large-scale hierarchical image database. In 2009 IEEE conference on computer vision and pattern recognition (pp. 248-255). Ieee.

ImageNet Large Scale Visual Recognition Challenge

Fei-Fei Li et al. 2010 (link)

Competition at:
Conference on Computer Vision and Pattern Recognition (CVPR)



Source: Quartz, link

What makes neural networks special?

Neural network learning is **representation learning**

Previous ML algorithms we discussed required us to manually determine feature transformations

Neural networks **learn** feature transformations

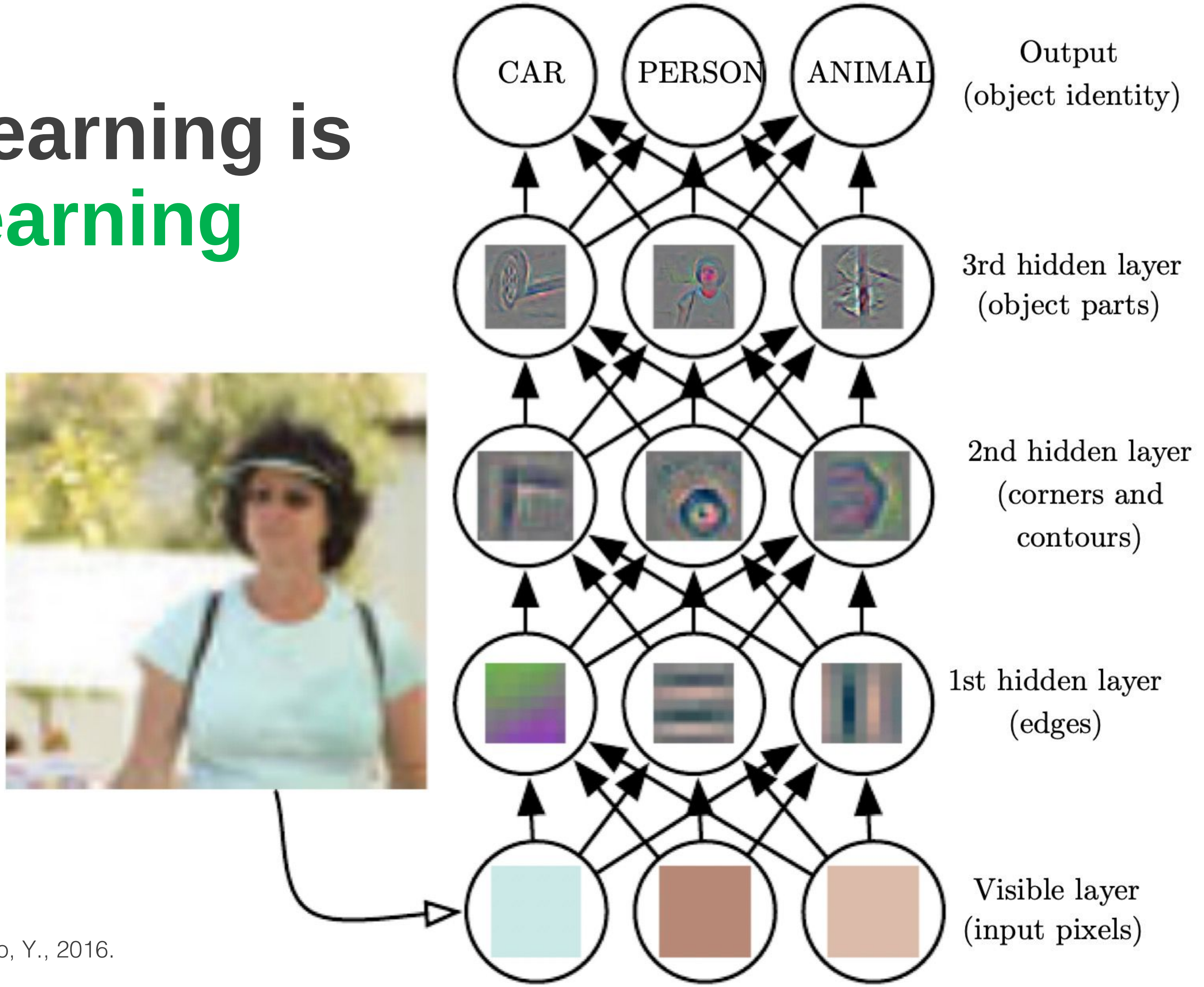


Image from Goodfellow, I., Bengio, Y., Courville, A. and Bengio, Y., 2016. Deep learning (Vol. 1, No. 2). Cambridge: MIT press.

What is a neural network and **how does it work**?

How do we **optimize model weights**?
(i.e. how do we fit our model to data)

What are the challenges of using neural networks?

Recall our goal in supervised learning

$$y = f(\boldsymbol{x}, \boldsymbol{w})$$

Labels

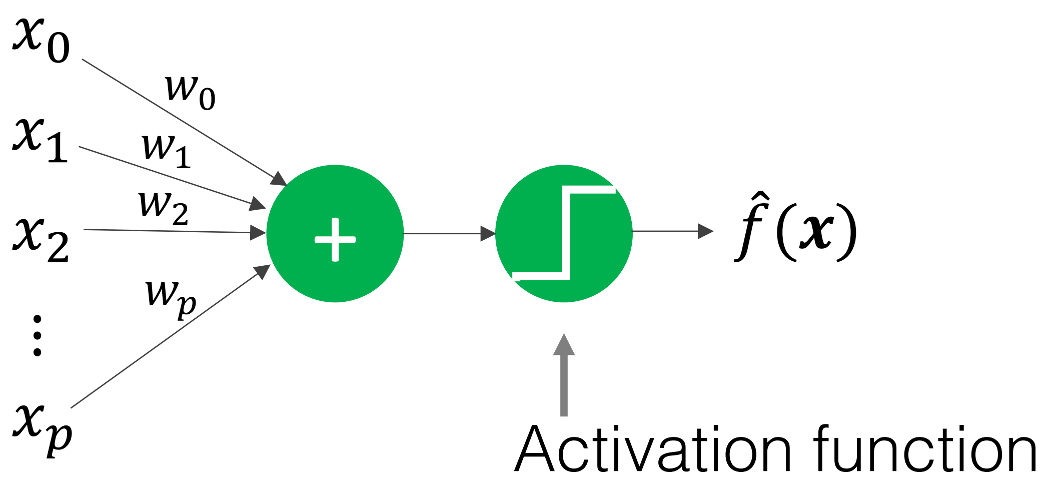
Parameter(s)

Model

Input Data

Perceptron

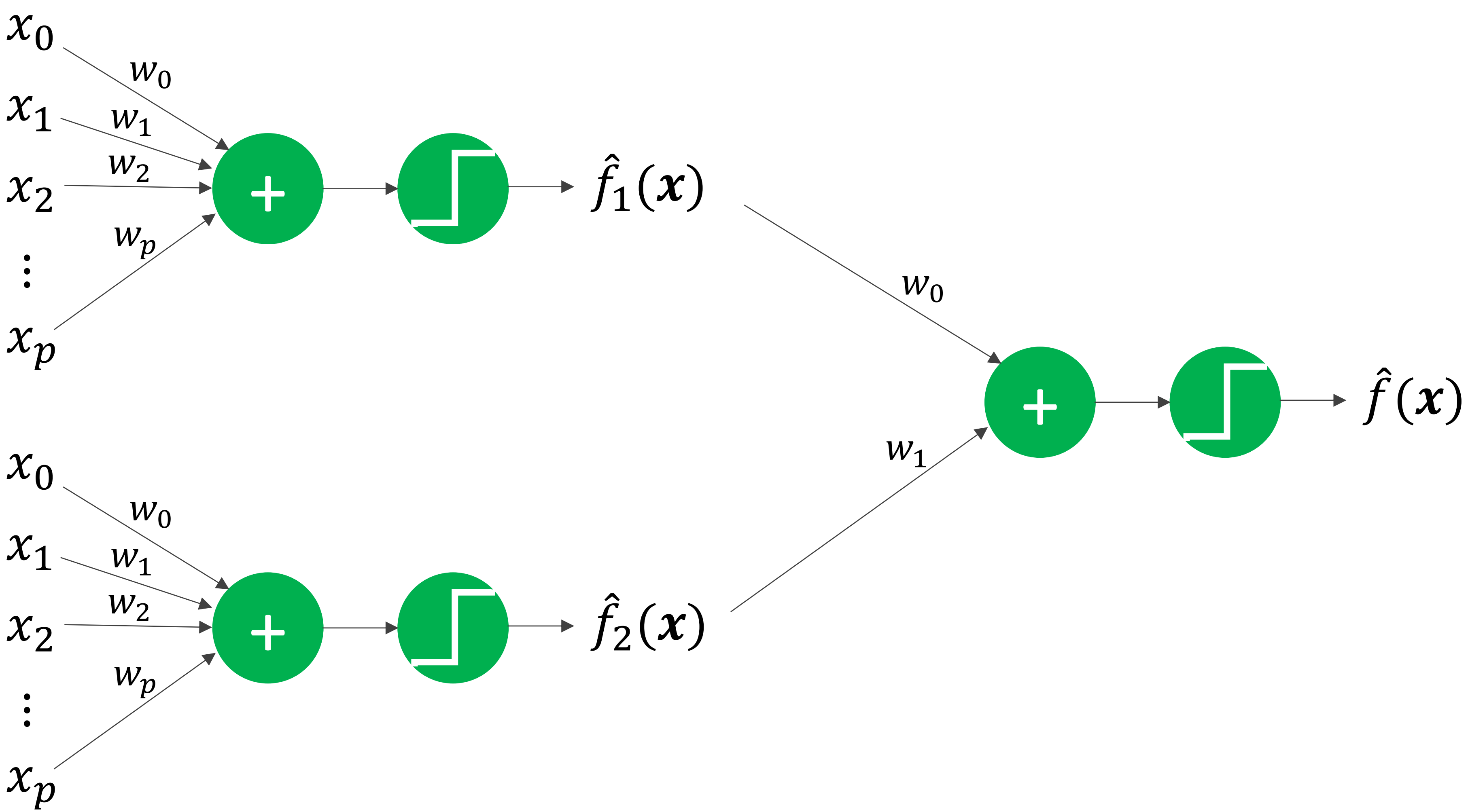
$$\hat{f}(\boldsymbol{x}) = sign\left(\sum_{i=0}^{p} w_i x_i\right)$$



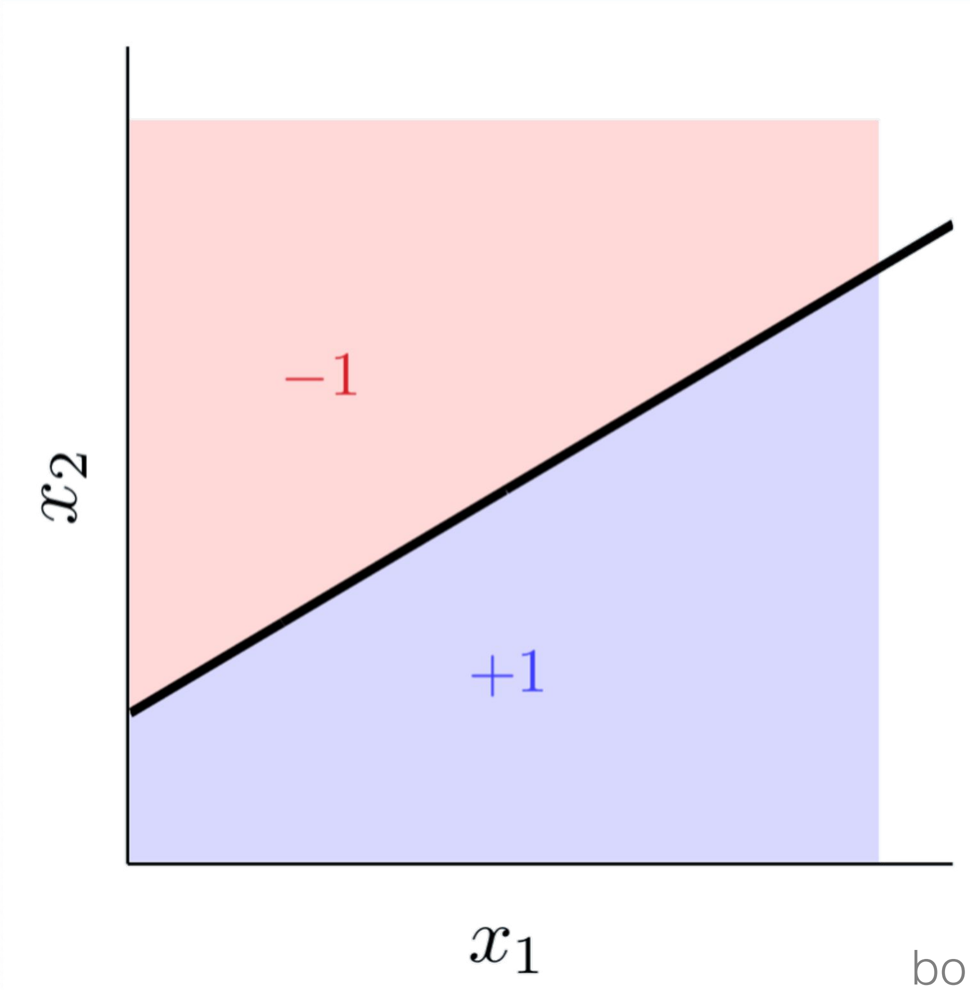
Source: Abu-Mostafa, Learning from Data, Caltech

Multilayer Perceptron

What if we stuck multiple perceptrons together?

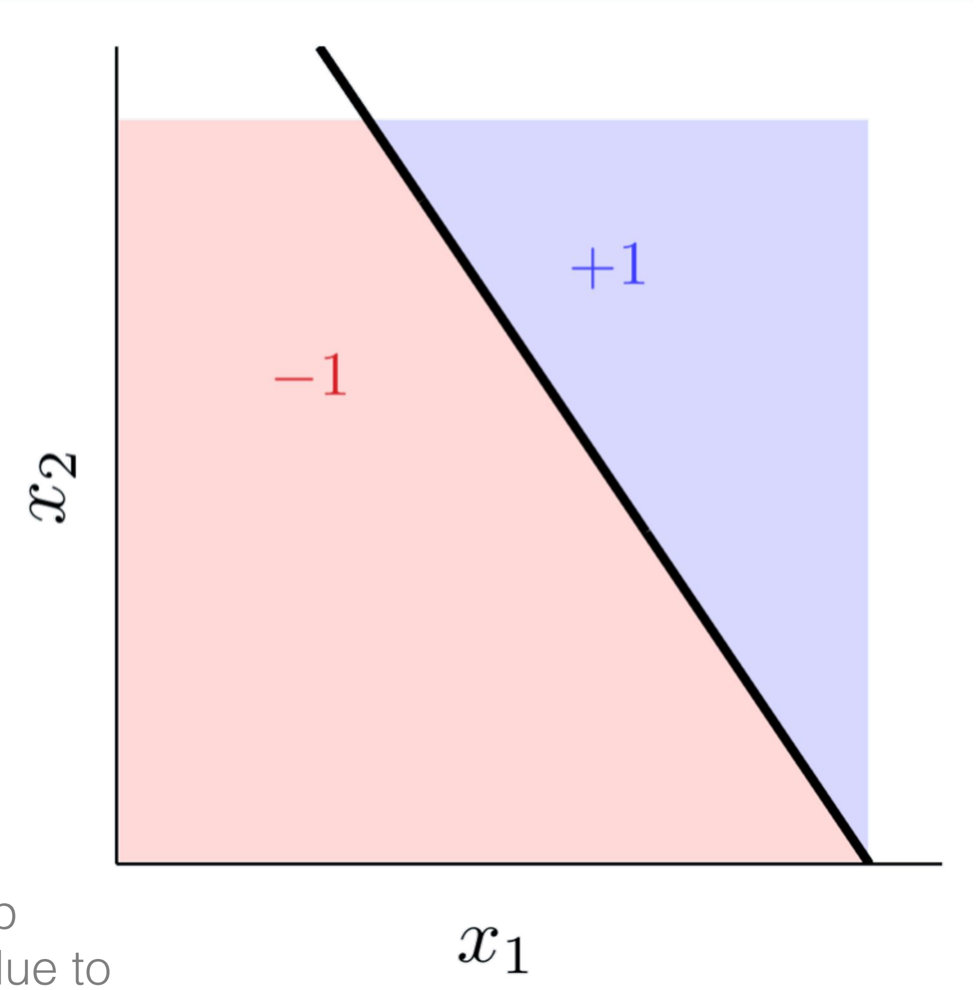


Perceptron #1



$\hat{f}_1(\boldsymbol{x}) = sign(\boldsymbol{w}_1^T \boldsymbol{x})$

Perceptron #2



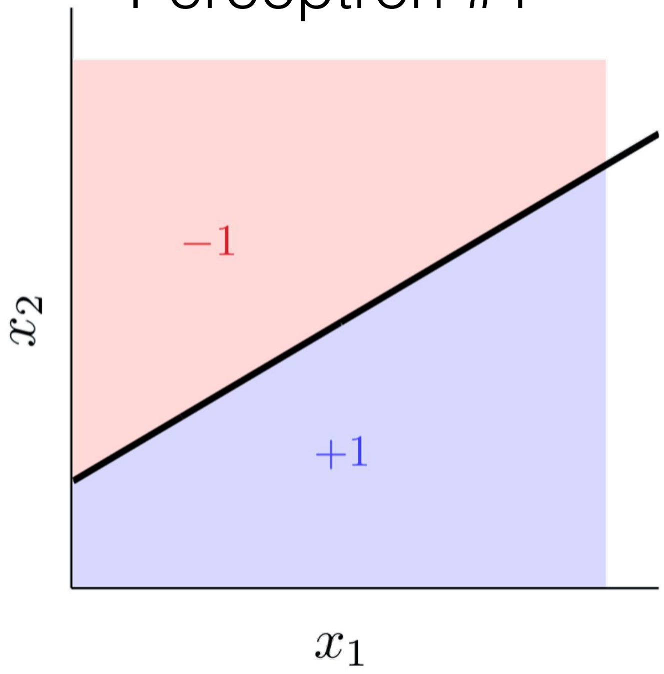
$\hat{f}_2(\boldsymbol{x}) = sign(\boldsymbol{w}_2^T \boldsymbol{x})$

The sharp boundary is due to our sign function

Source: Abu-Mostafa, Learning from Data, Caltech

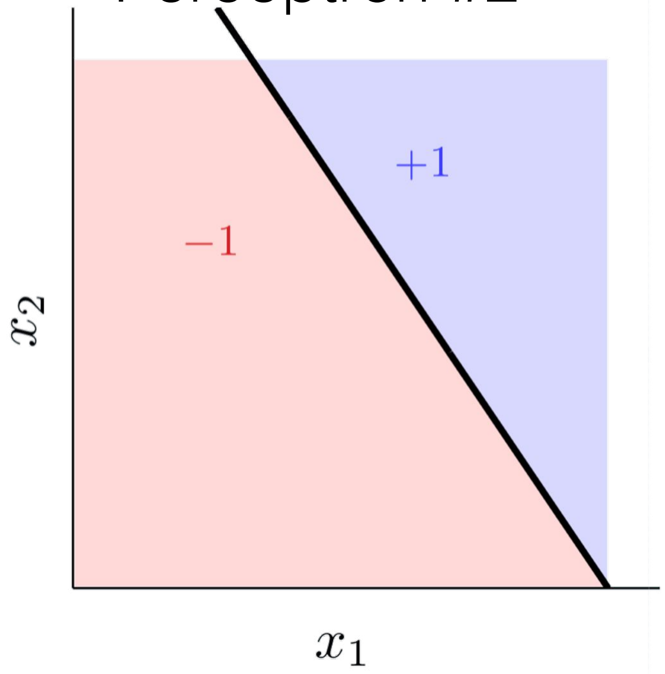
Multilayer perceptron: $\hat{f}(\boldsymbol{x}) = \begin{cases} +1, & \hat{f}_1(\boldsymbol{x}) \neq \hat{f}_2(\boldsymbol{x}) \\ -1, & \hat{f}_1(\boldsymbol{x}) = \hat{f}_2(\boldsymbol{x}) \end{cases}$

Perceptron #1

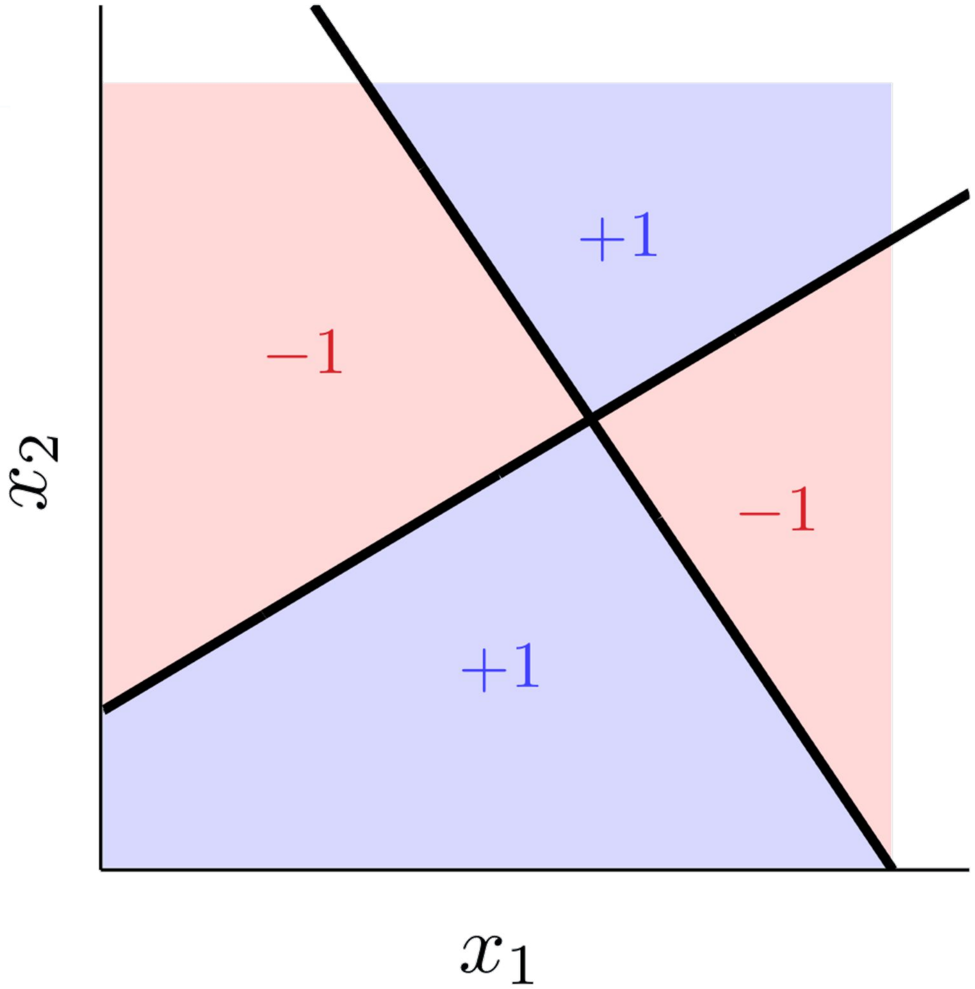


$$\hat{f}_1(\boldsymbol{x}) = sign(\boldsymbol{w}_1^T \boldsymbol{x})$$

Perceptron #2

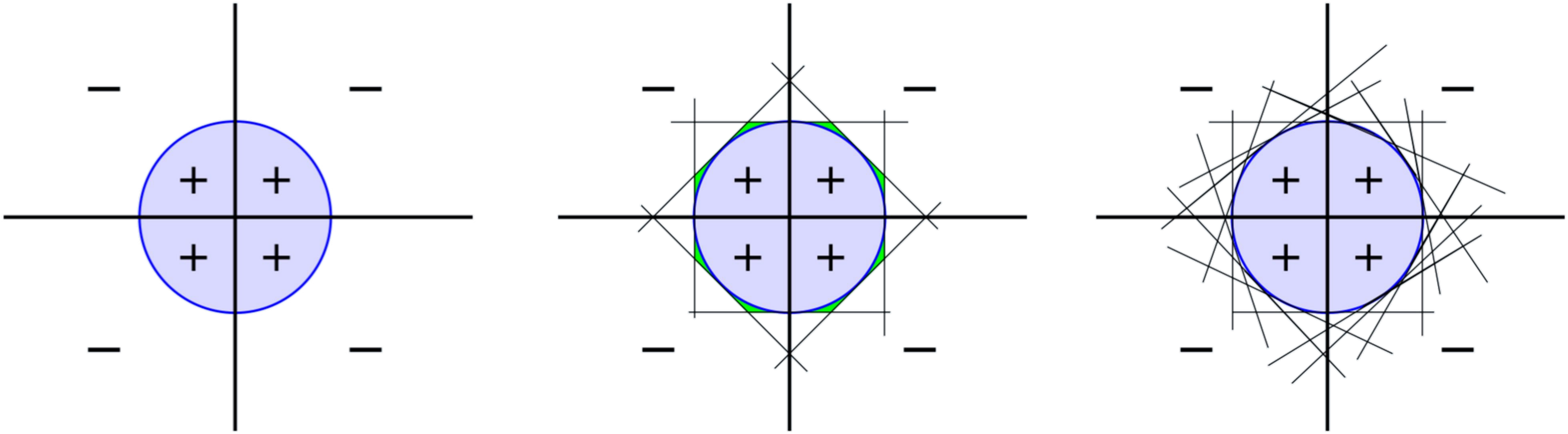


$$\hat{f}_2(\boldsymbol{x}) = sign(\boldsymbol{w}_2^T \boldsymbol{x})$$



Source: Abu-Mostafa, Learning from Data, Caltech

Multilayer Perceptron



Target | 8 perceptrons | 16 perceptrons

The more nodes/neurons, the more flexible is the model

Source: Abu-Mostafa, Learning from Data, Caltech

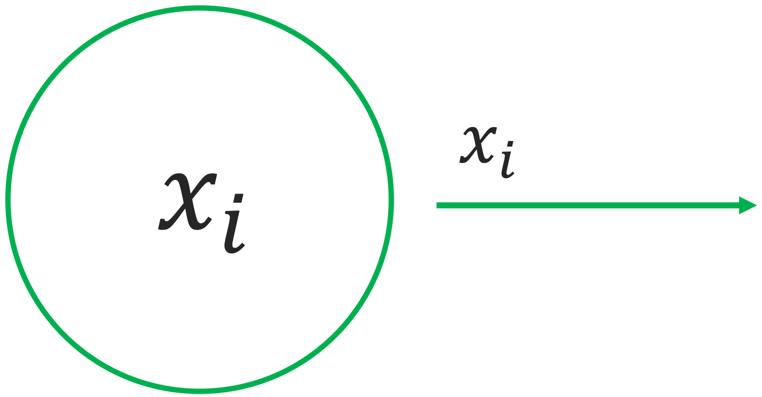
Universal function approximation

"A **feedforward network** with a single layer is sufficient to represent **any function**, but the layer may be infeasibly large and may fail to learn and generalize correctly."

Ian Goodfellow, Deep Learning

Creator of generative adversarial networks

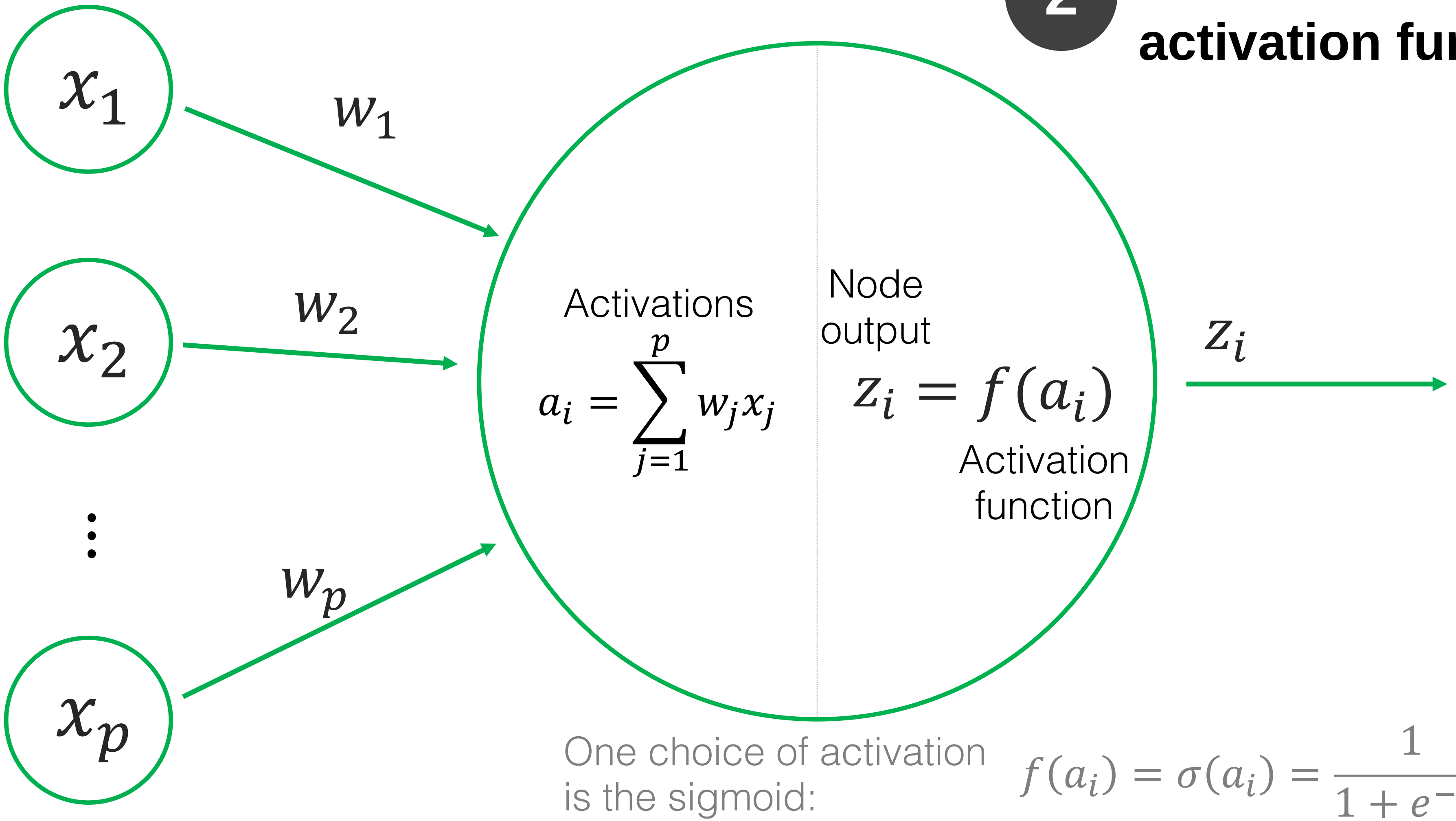
Input nodes / neurons



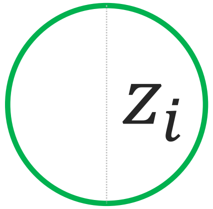
Simply passes the input value to the next layer

Hidden & output nodes

1. Calculate the **activations**: linear combinations of weights and the last layer's output
2. Calculate node output: apply the **activation function** to the activations

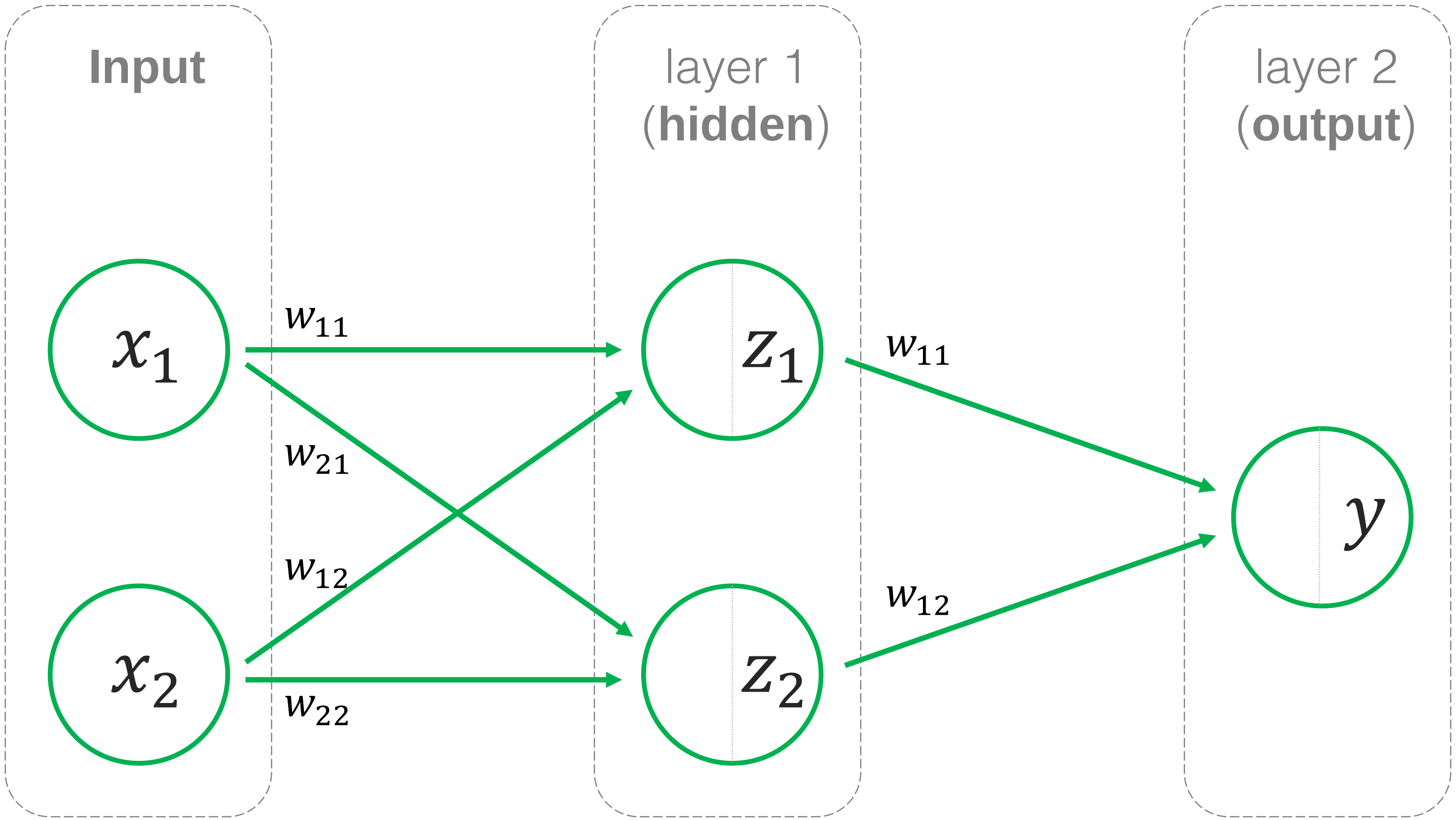


Represented as:



One choice of activation is the sigmoid: $f(a_i) = \sigma(a_i) = \dfrac{1}{1+e^{-a_i}}$

Simple Neural Network



$$w_{ij}^{(k)}$$

Layer k

From node j
(in the last layer)

to node i
(in the next layer)

Notational shorthand:
(a more precise
alternative notation)

$w_{ij} = w_{ij}^{(1)}$ $\quad z_i = z_i^{(1)}$ $\quad w_{ij} = w_{ij}^{(2)}$ $\quad y = z_1^{(2)}$

Forward Propagation

Calculating the output from input

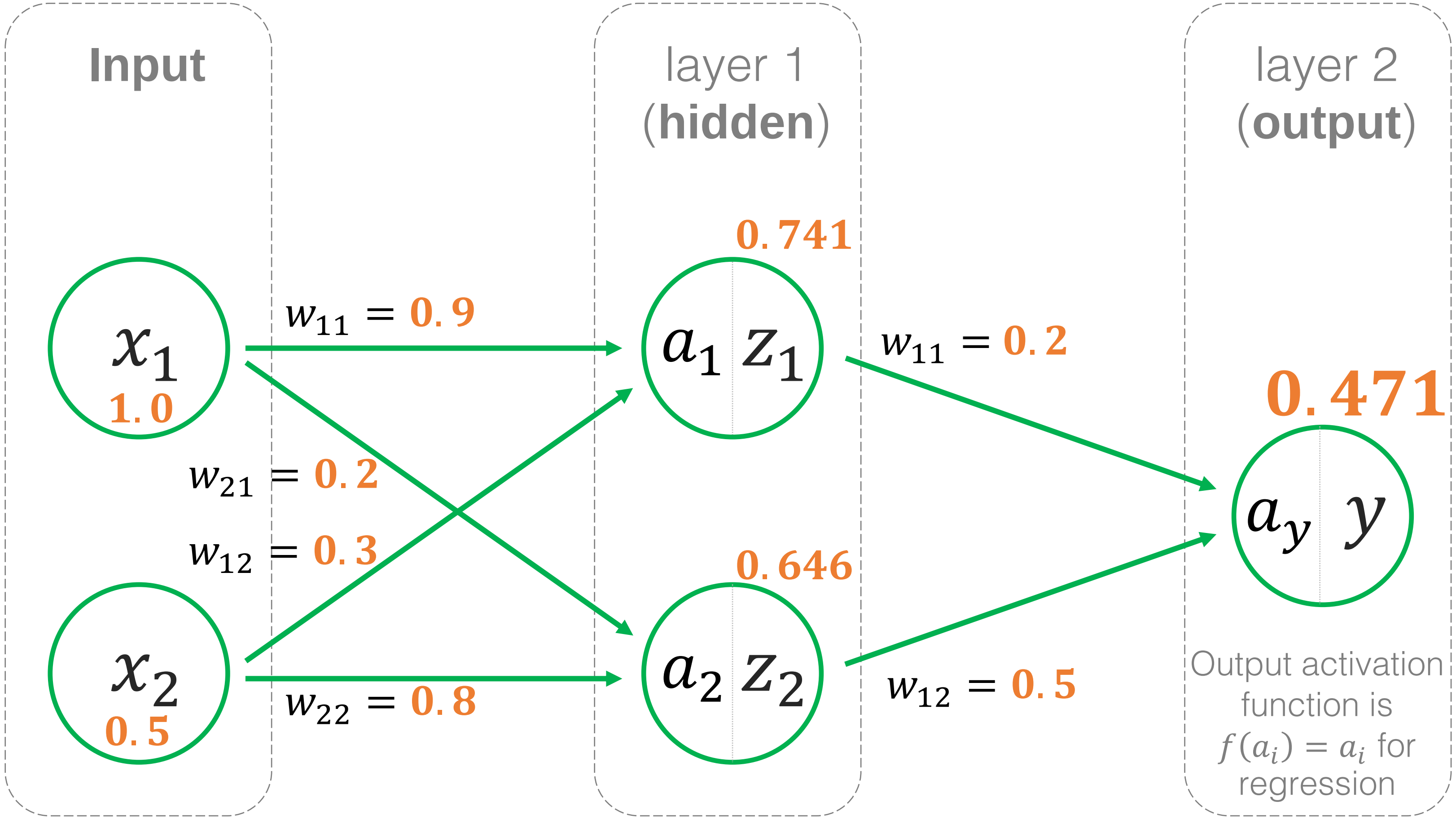
Hidden layer calculations

$$a_1 = (0.9)(1.0) + (0.3)(0.5) = 1.05$$

$$a_2 = (0.2)(1.0) + (0.8)(0.5) = 0.6$$

$$z_1 = \sigma(a_1) = \sigma(1.05) = 0.741$$

$$z_2 = \sigma(a_2) = \sigma(0.6) = 0.646$$



Output layer calculations

$$a_y = (0.2)(0.741) + (0.5)(0.646) = 0.471$$

$y = a_y = 0.471$ Regression

Alternatively…

$y = \sigma(a_y) = \sigma(0.471) = 0.616$

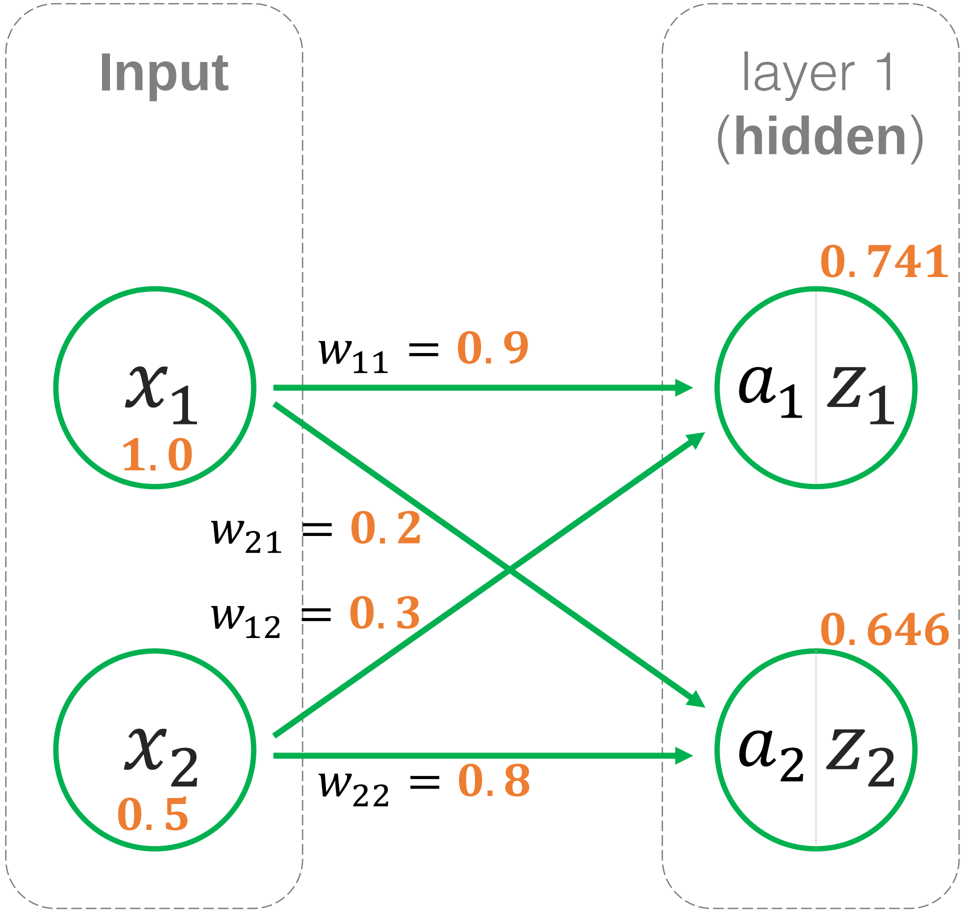
Classification

$$\sigma(a_i) = \frac{1}{1 + e^{-a_i}}$$

Rashid, Make Your Own Neural Network

Forward Propagation

Calculating the output from input



Hidden layer matrix calculations

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad \boldsymbol{a} = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \quad \boldsymbol{z} = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$$

$$\boldsymbol{W} = \begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{bmatrix}$$

The weights INTO node z_1

The weights INTO node z_2

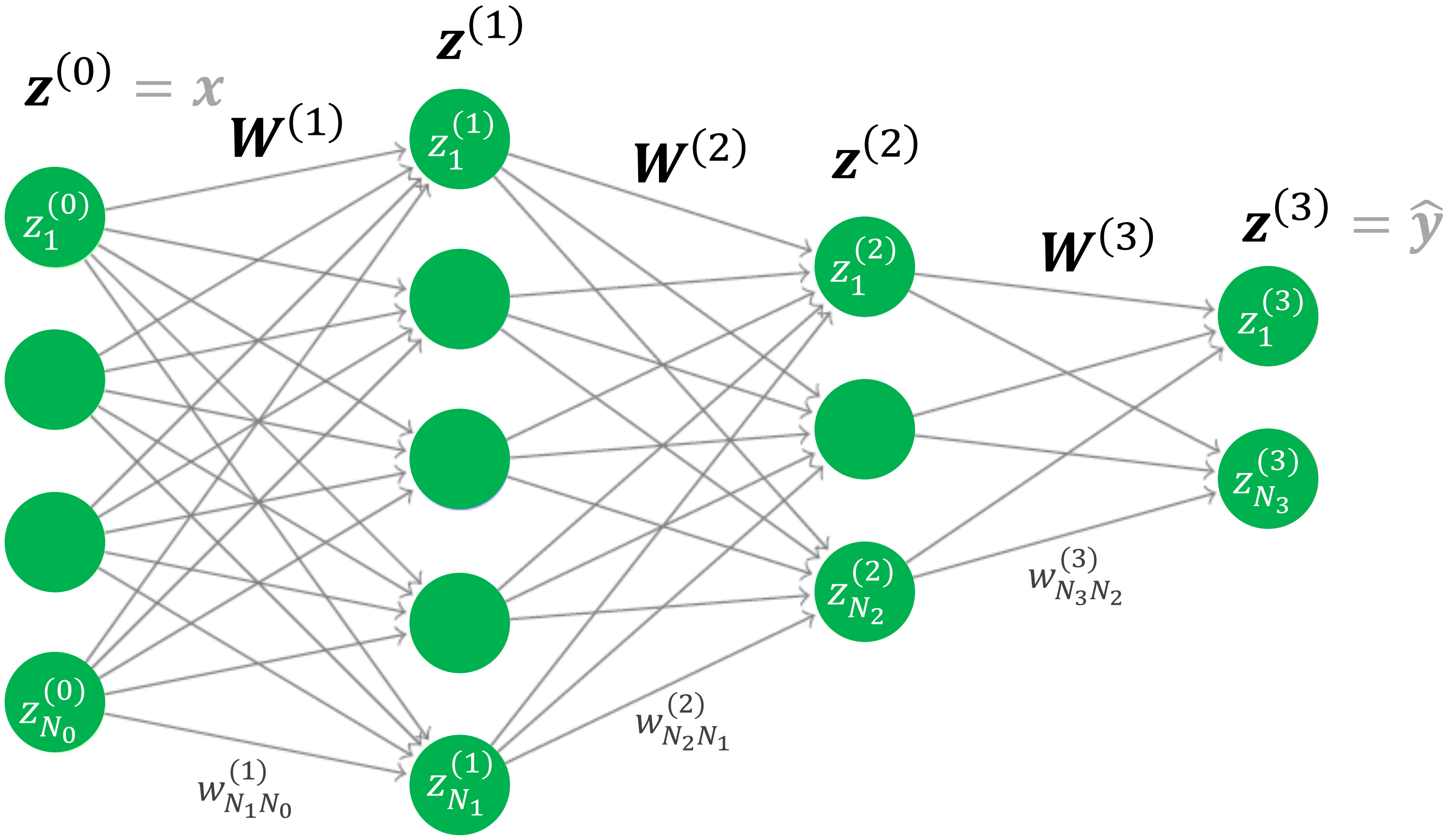
$$\boldsymbol{a} = \boldsymbol{W}\boldsymbol{x} = \begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$= \begin{bmatrix} w_{11}x_1 + w_{12}x_2 \\ w_{21}x_1 + w_{22}x_2 \end{bmatrix}$$

$$\boldsymbol{z} = \sigma(\boldsymbol{a}) = \begin{bmatrix} \sigma(w_{11}x_1 + w_{12}x_2) \\ \sigma(w_{21}x_1 + w_{22}x_2) \end{bmatrix}$$

Forward Propagation

Example neural network with $L = 3$ layers and the ith layer has N_i nodes



Simple steps for forward propagation:

$$\boxed{\begin{array}{l}\text{For } i = 1 \text{ to } L-1: \\ \quad \mathbf{z}^{(i)} = \sigma\left(\mathbf{W}^{(i)} \mathbf{z}^{(i-1)}\right)\end{array}}$$

Where:

$$\mathbf{z}^{(0)} = \mathbf{x}$$

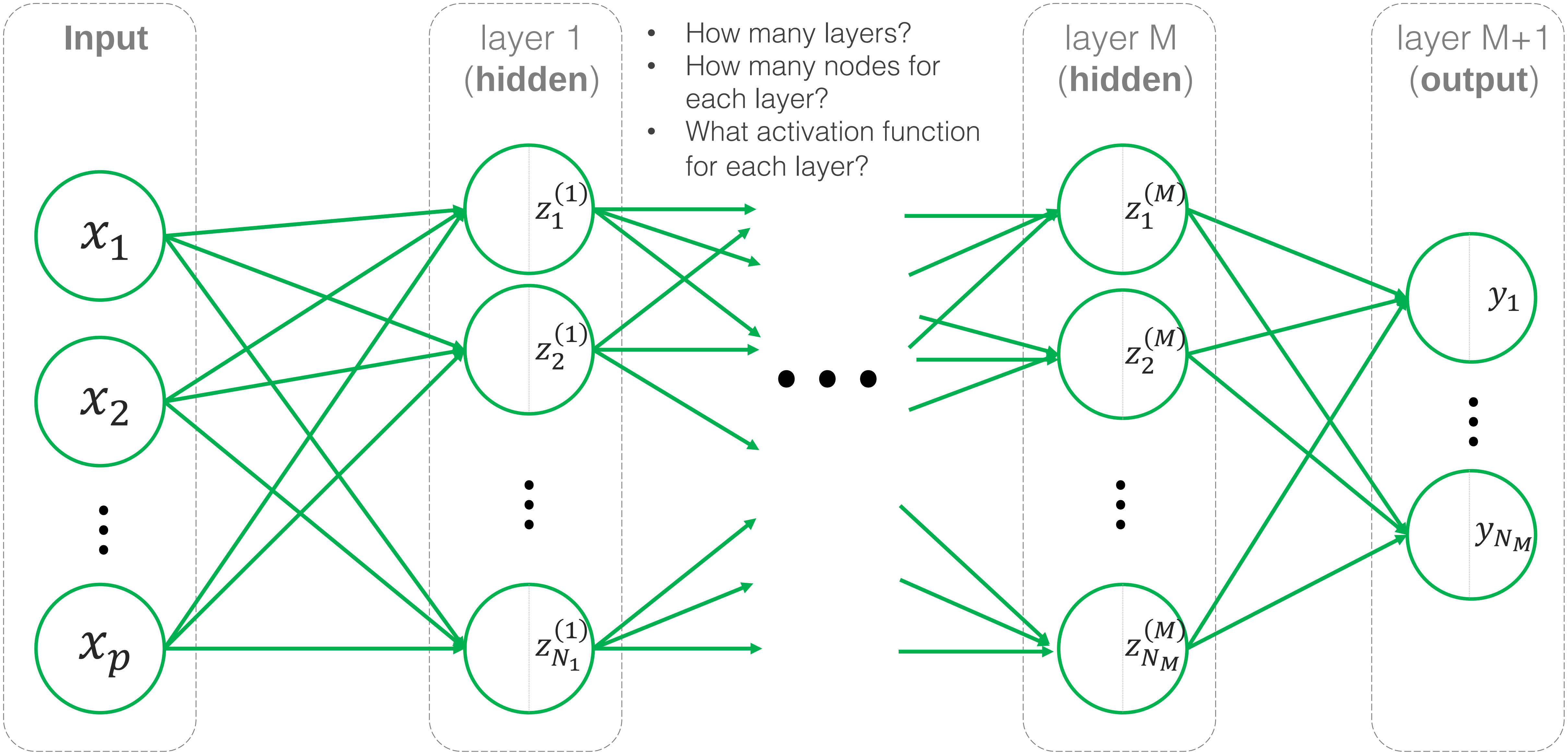
$$\hat{\mathbf{y}} = \mathbf{z}^{(L)}$$

Prediction error is measured:

$$E_n = \frac{1}{2}(\hat{y}_n - y_n)^2$$

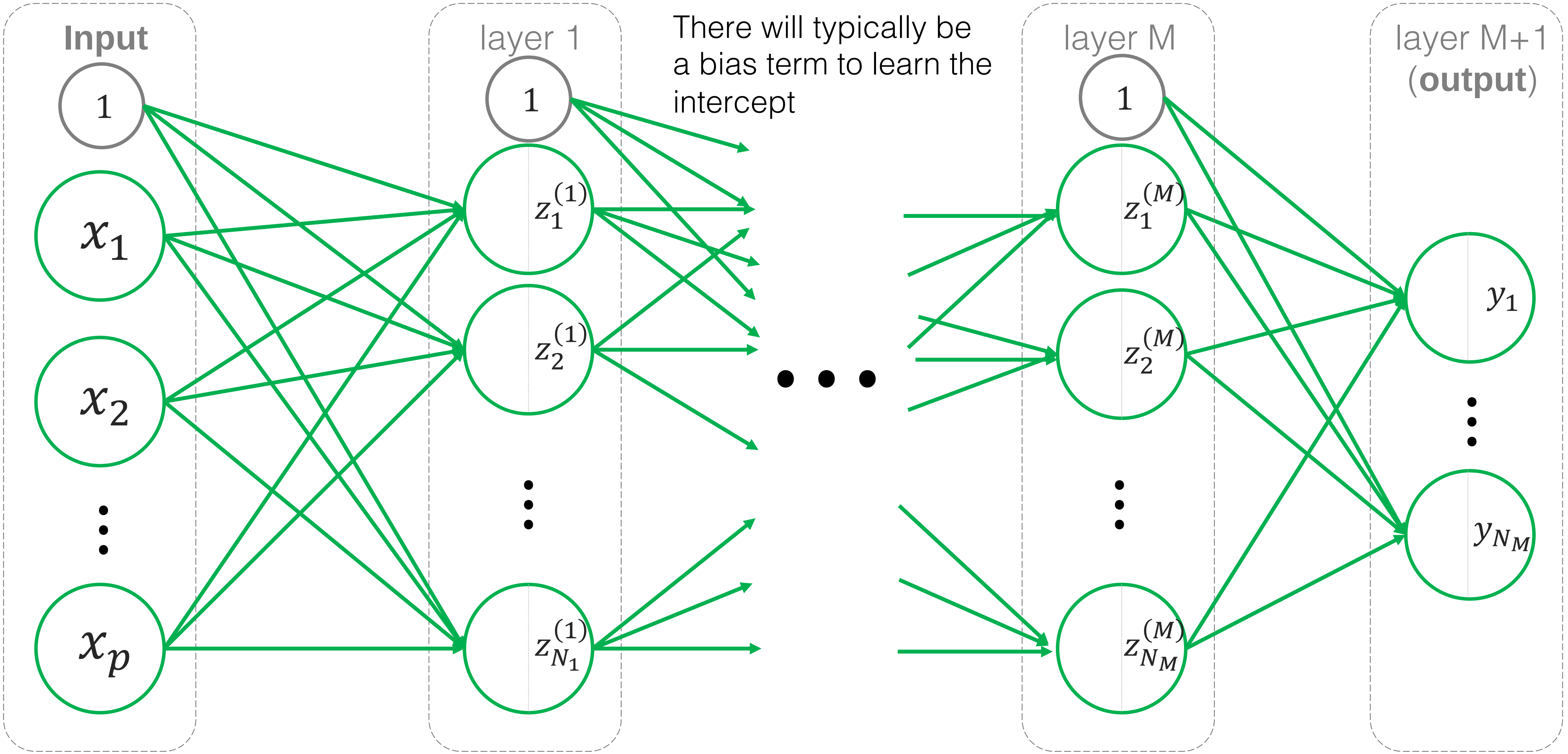
Sudeep Raja, A Derivation of Backpropagation in Matrix Form

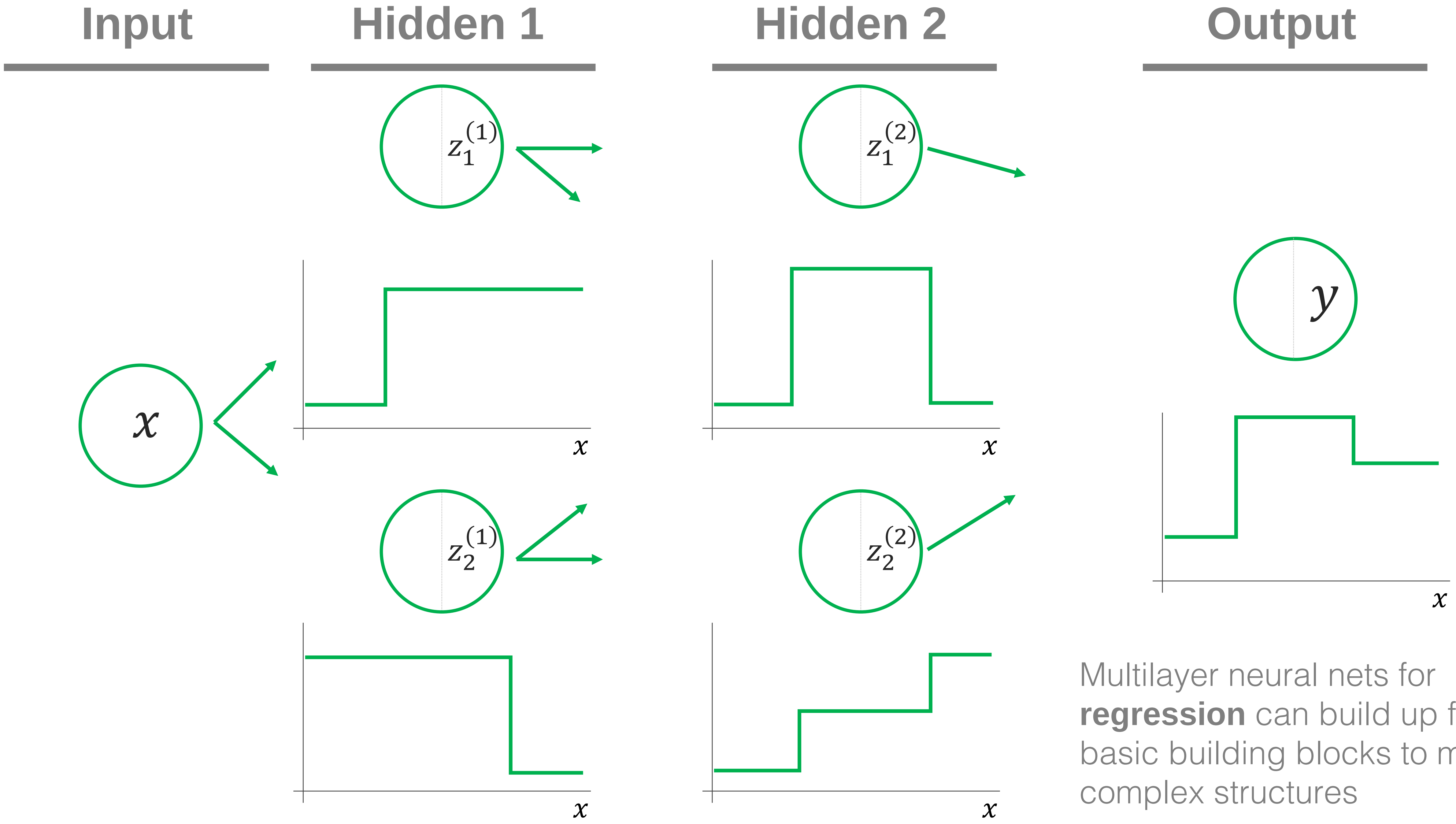
Neural networks can be customized



- How many layers?
- How many nodes for each layer?
- What activation function for each layer?

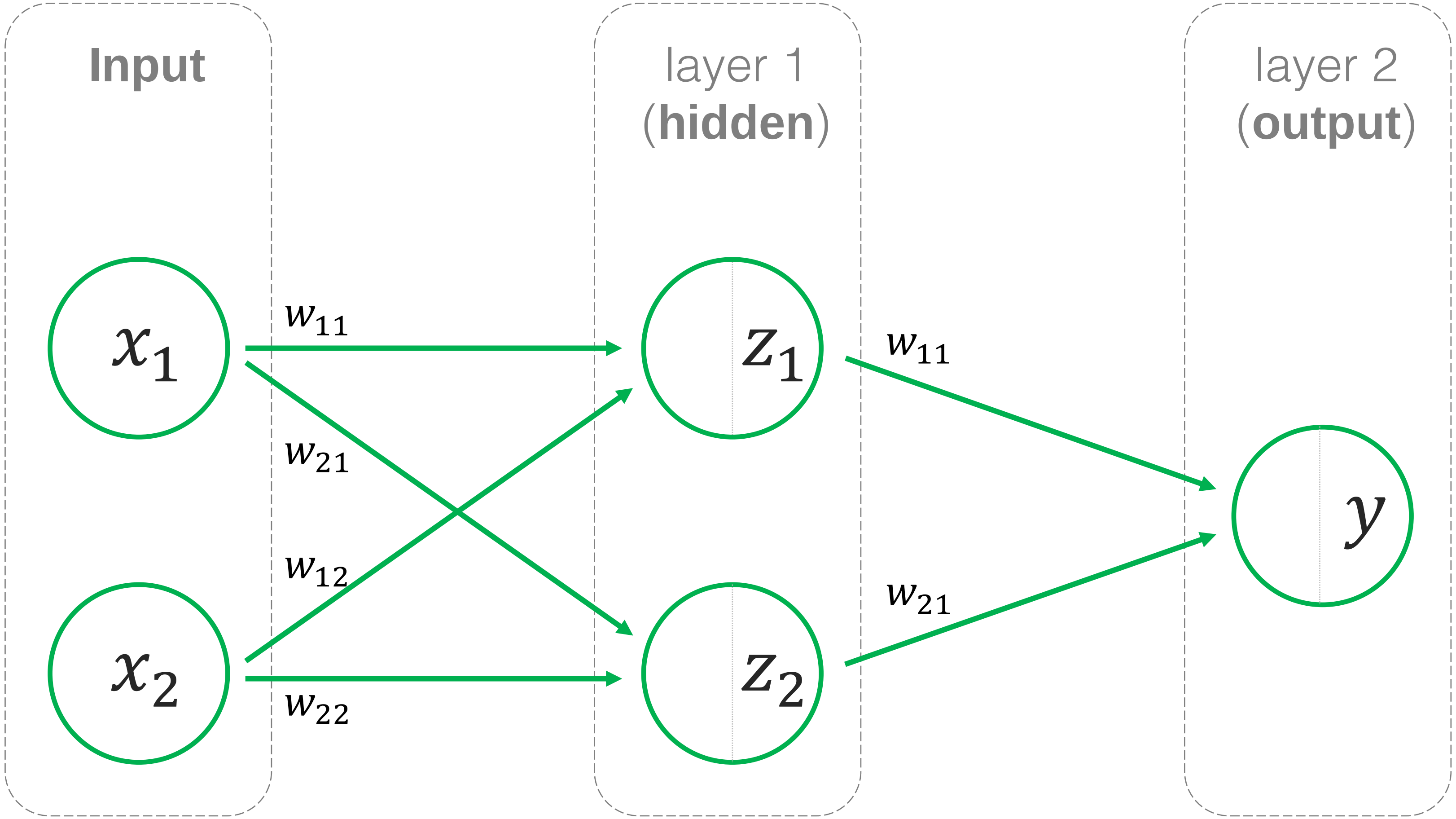
Neural networks can be customized





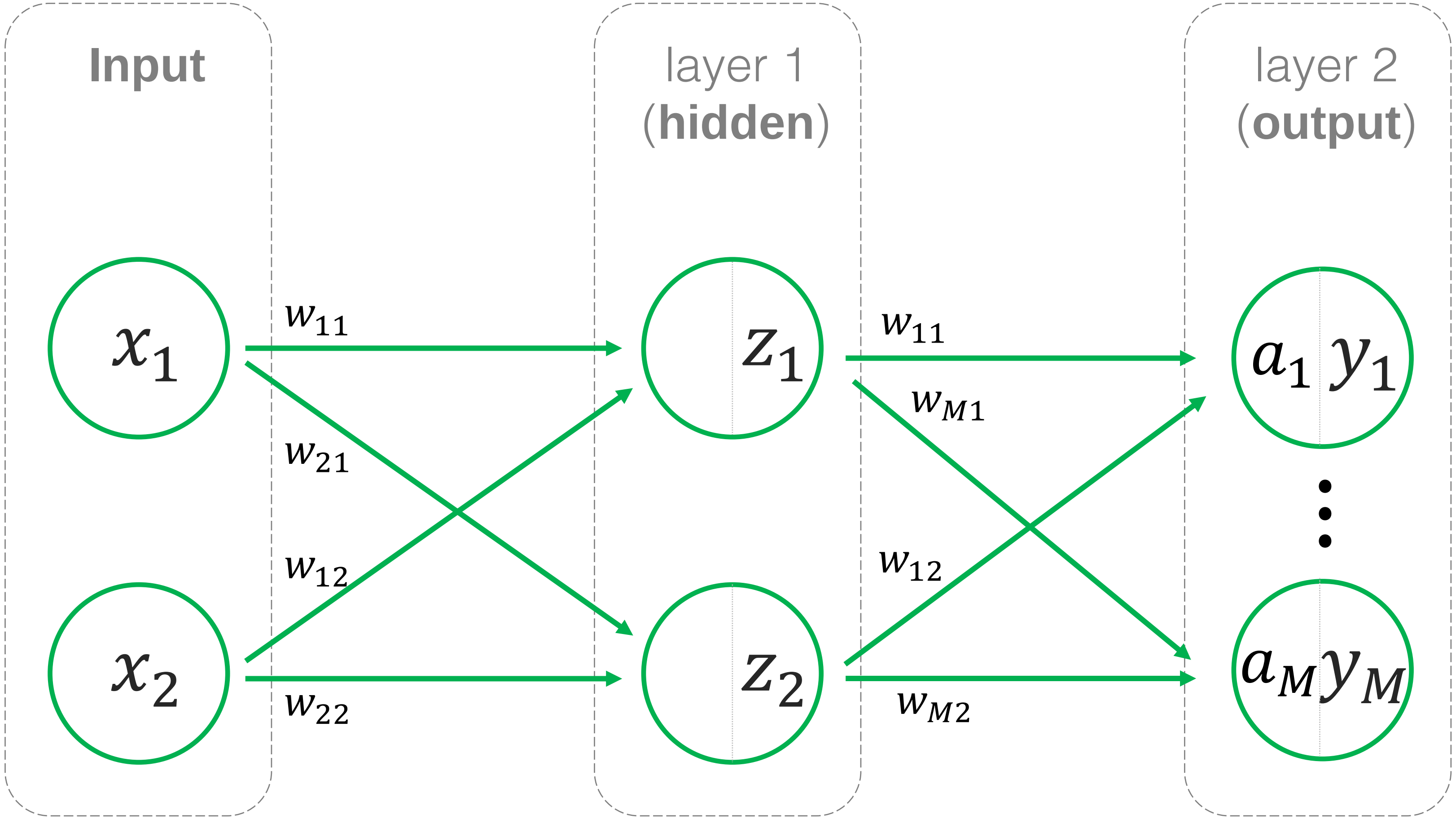
Multilayer neural nets for **regression** can build up from basic building blocks to more complex structures

From binary to multiclass classification



For **binary classification** with a sigmoid activation function, the output is between zero and one, so threshold this value to assign the class

From binary to multiclass classification



For **multiclass problems**, we can have multiple outputs and use a softmax function:
(a generalization of the sigmoid / logistic function)

$$y_i = g(a_i) = \frac{e^{a_i}}{\sum_{n=1}^{M} e^{a_n}}$$

Choose the largest y value as the predicted class

Softmax

Generalization of the logistic function to multiple dimensions

Output activations

a_i

$$\begin{bmatrix} 5.1 \\ 4.2 \\ -3.1 \\ 0.7 \end{bmatrix}$$

Activation Function

$\text{softmax}(a_i)$

Softmax

$$\frac{e^{a_i}}{\sum_{n=1}^{M} e^{a_n}}$$

Output

y_i

$$\begin{bmatrix} 0.7046 \\ 0.2865 \\ 0.0002 \\ 0.0087 \end{bmatrix}$$

Always sums to 1
(normalizes to be a probability distribution)

Next time…

What is a neural network and **how does it work**?

How do we **optimize model weights**?
(i.e. how do we fit our model to data)

What are the challenges of using neural networks?