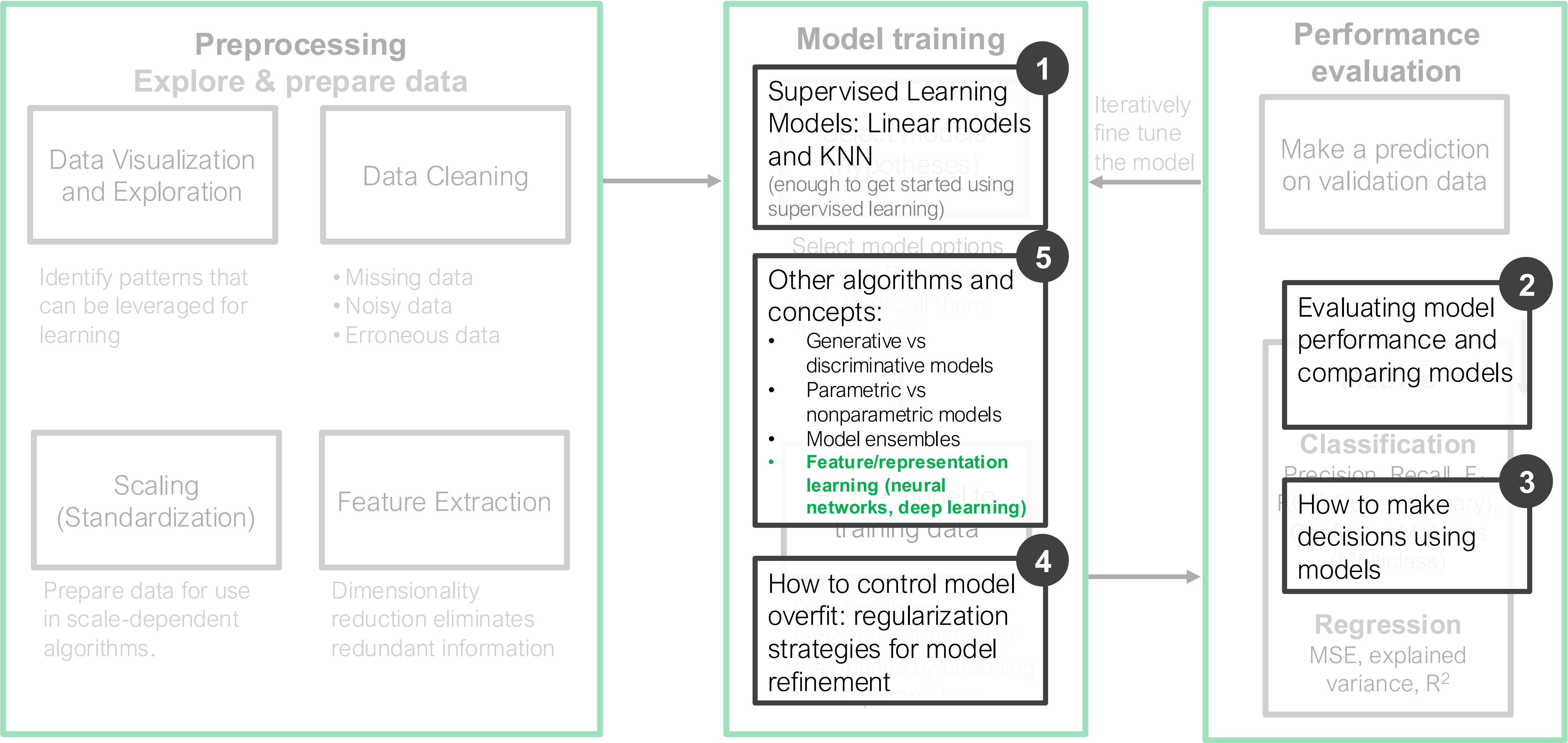
Neural Networks I

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)

Select model options

5 Other algorithms and concepts:

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

training data

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

Classification

Precision, Recall, F

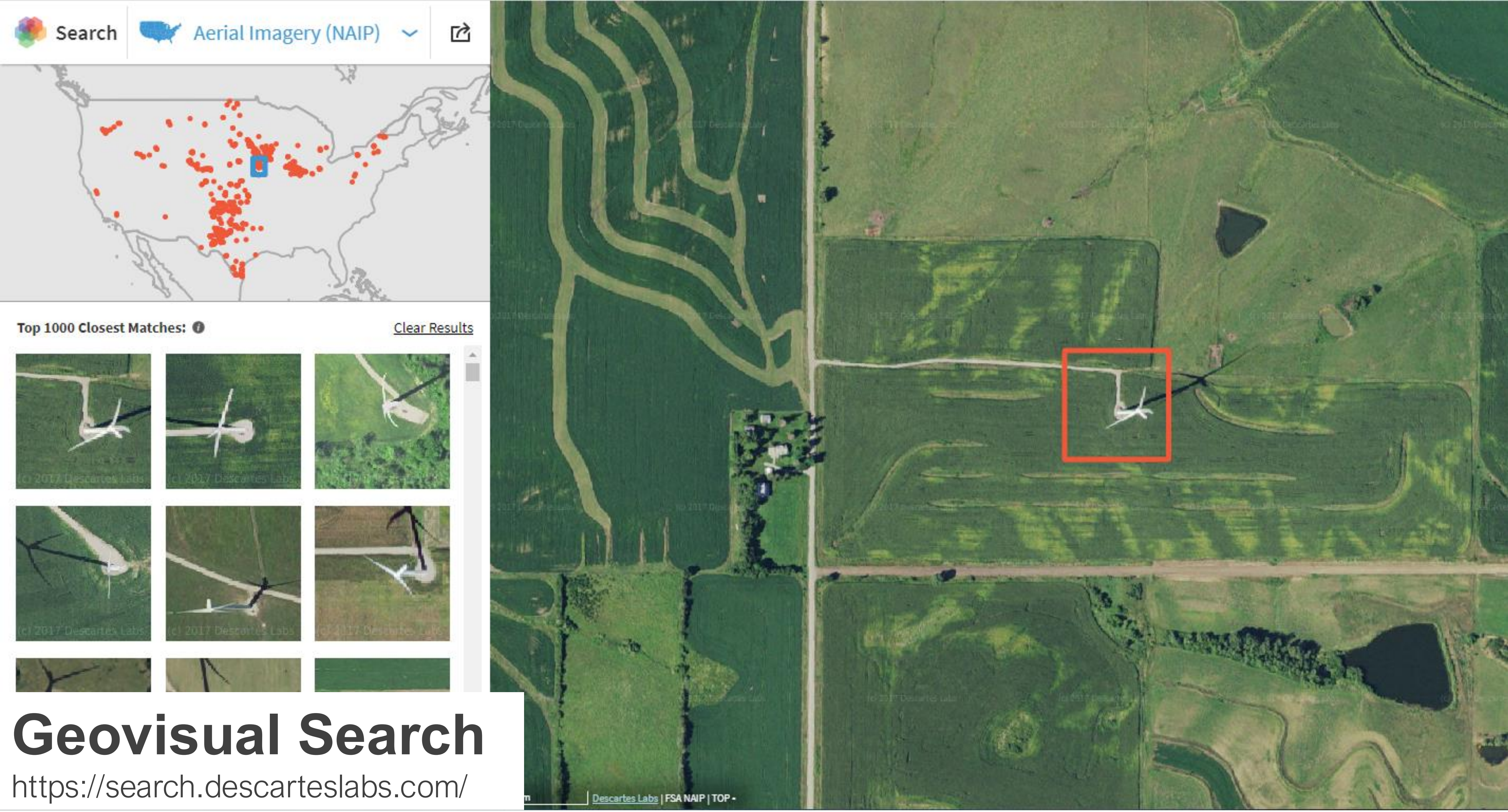
3 How to make decisions using models

Regression

MSE, explained variance, R^2

What’s the hype around neural networks?

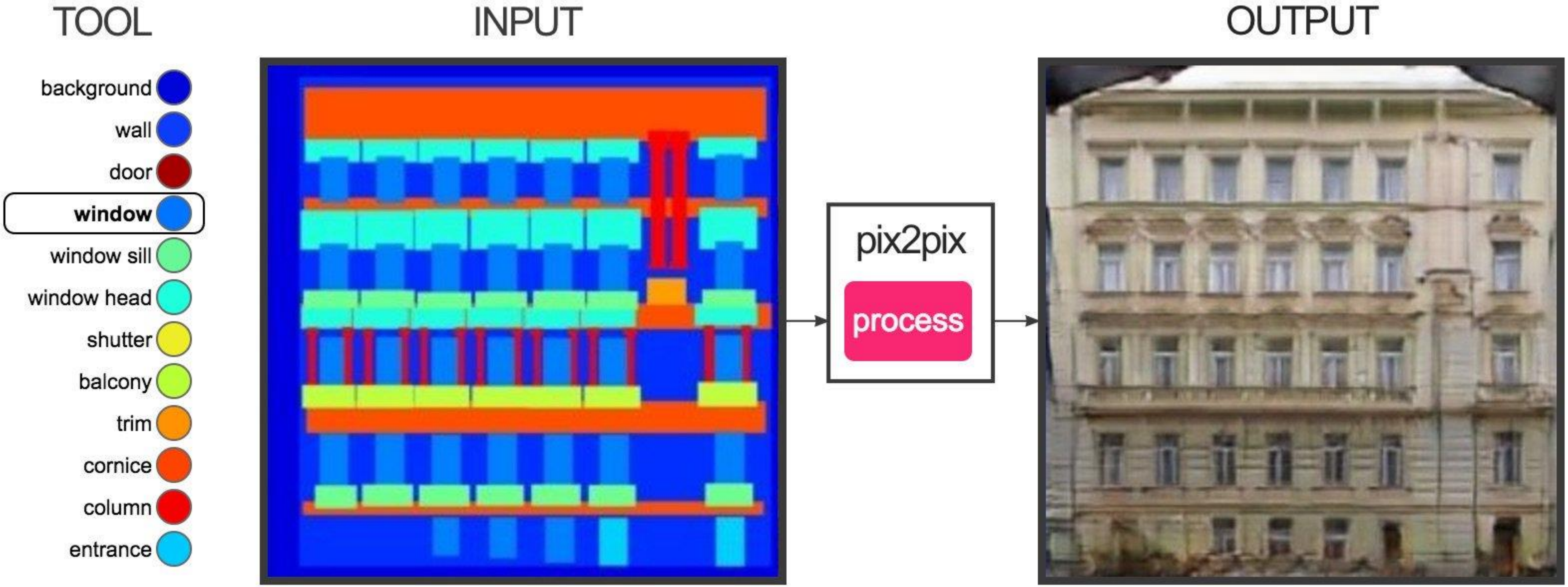
Character/handwriting recognition
Self-driving cars
Natural language processing and translation
Speech recognition
Medical devices, diagnosis, and treatment
Materials development
Automated financial trading systems
Industrial automation
Computer vision applications…



Geovisual Search

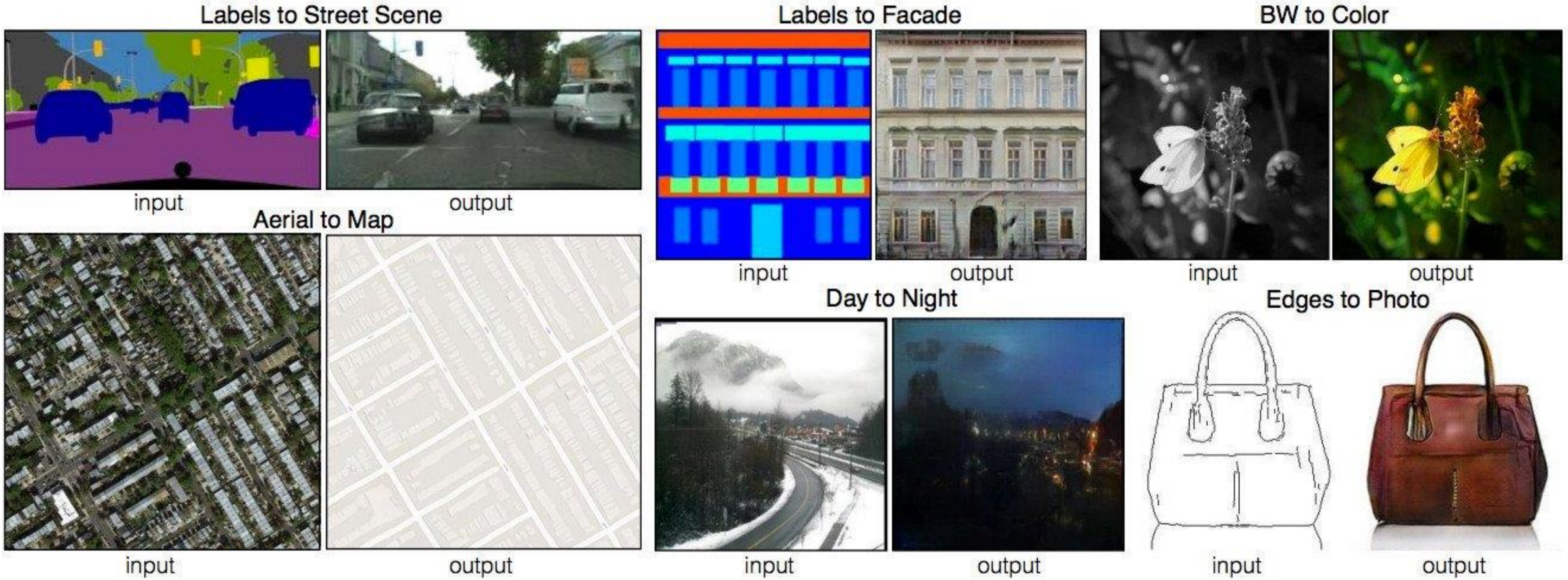
https://search.descarteslabs.com/

Image-to-image translation



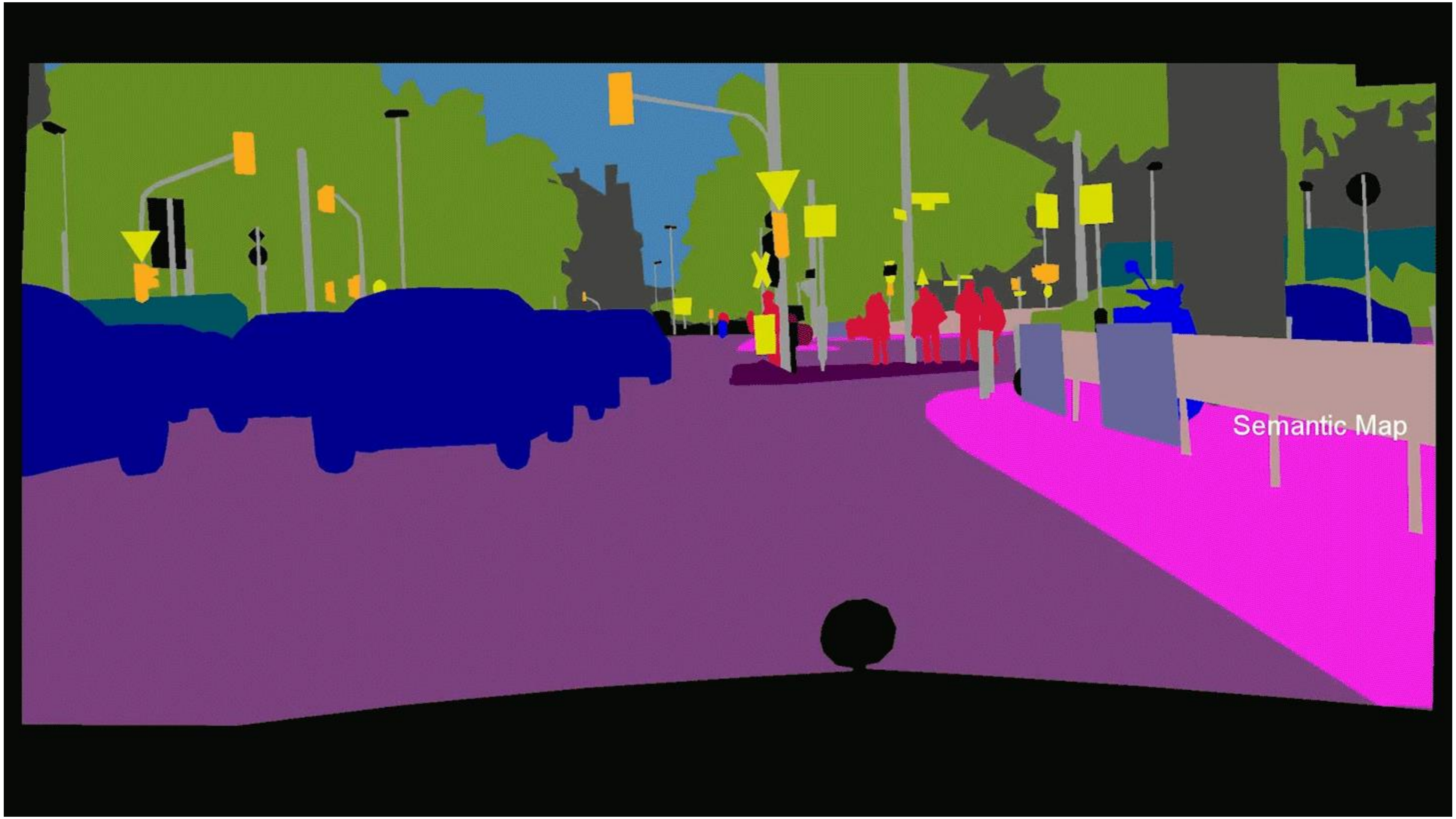
Isola, Phillip, et al. "Image-to-image translation with conditional adversarial networks." arXiv preprint (2017).

Image-to-image translation



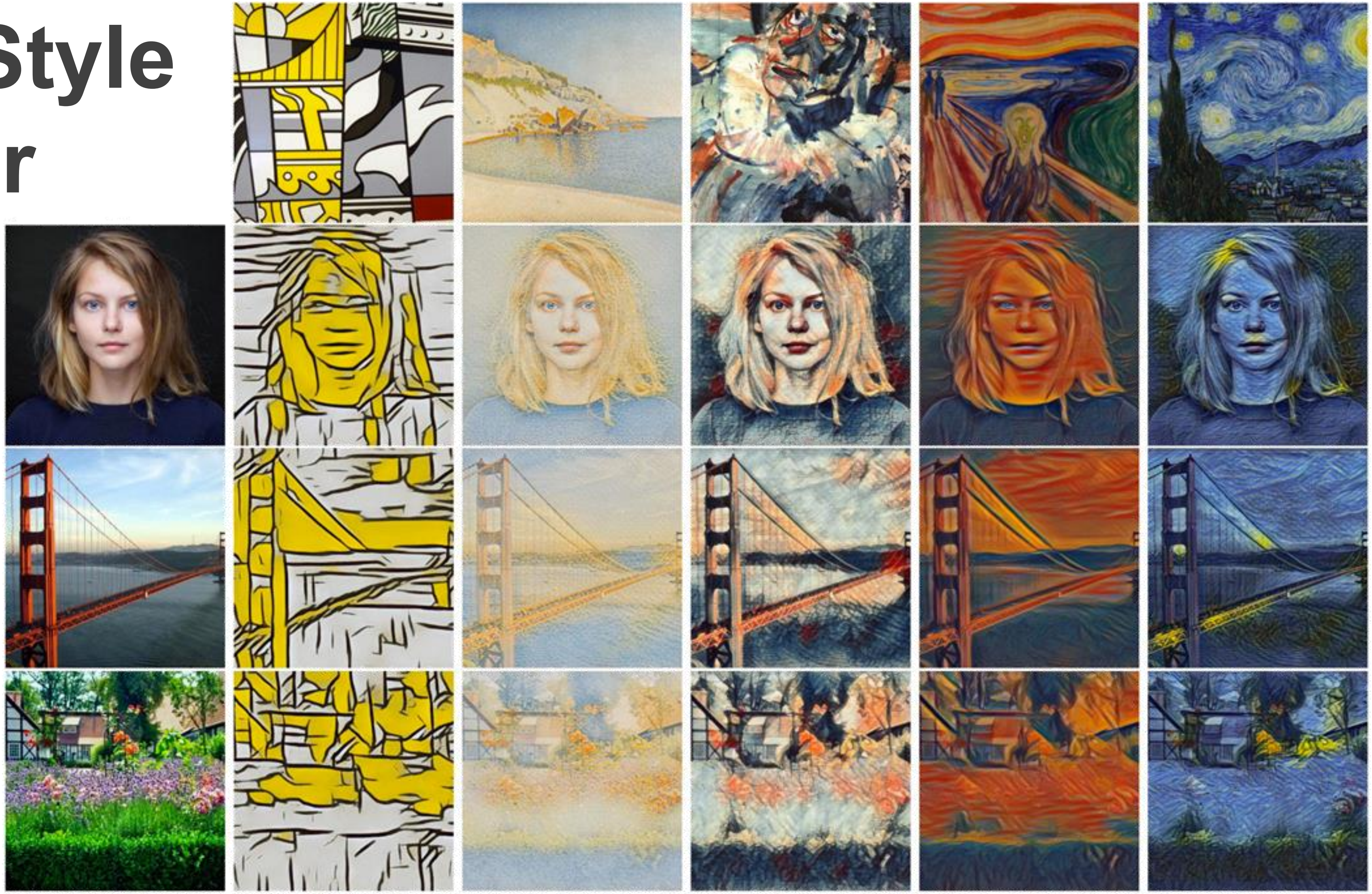
Isola, Phillip, et al. "Image-to-image translation with conditional adversarial networks." arXiv preprint (2017).

Image-to-image translation



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

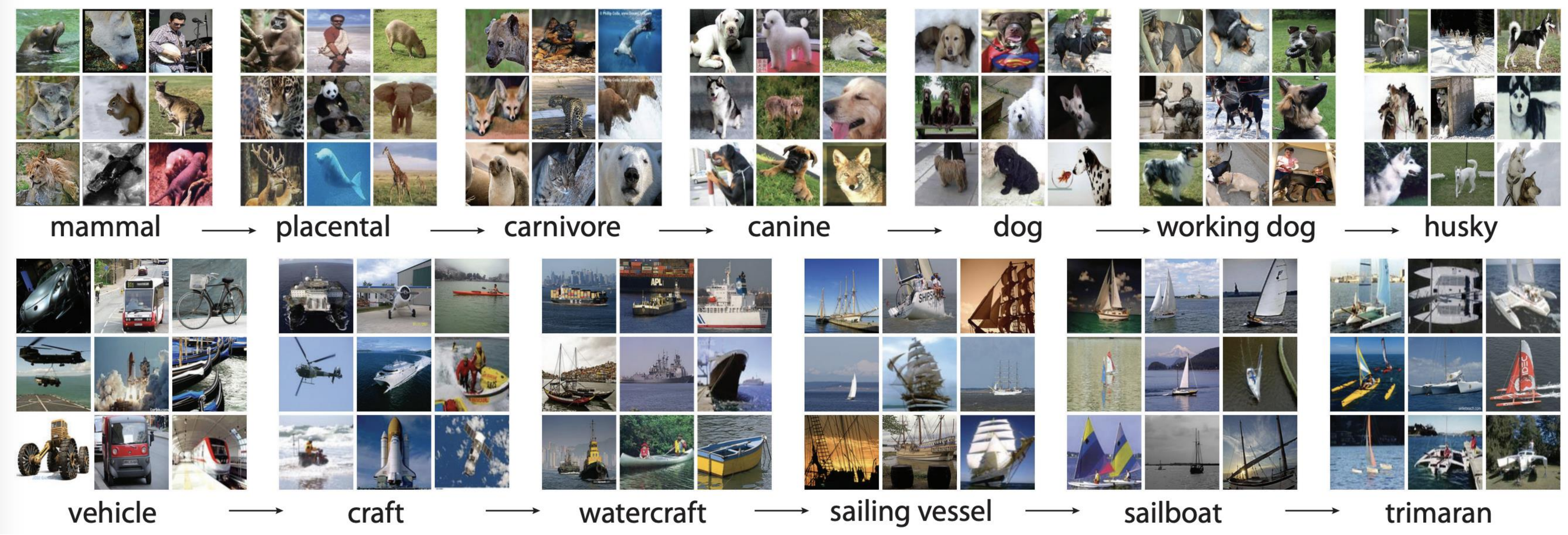
Image Style Transfer



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

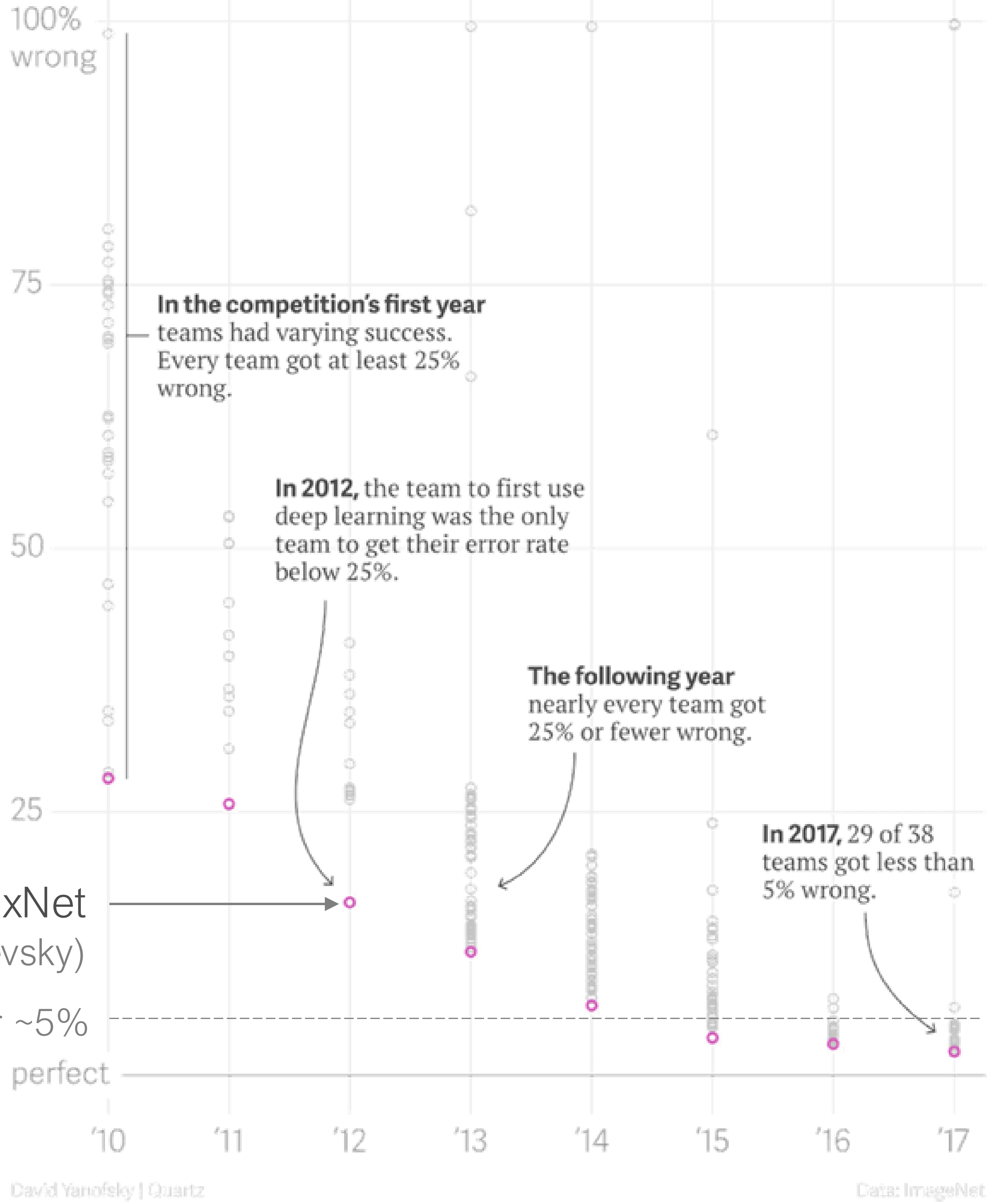

mammal → placental → carnivore → canine → dog → working dog → husky
vehicle → craft → watercraft → sailing vessel → sailboat → trimaran

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)



In the competition's first year teams had varying success. Every team got at least 25% wrong.

In 2012, the team to first use deep learning was the only team to get their error rate below 25%.

The following year nearly every team got 25% or fewer wrong.

In 2017, 29 of 38 teams got less than 5% wrong.

AlexNet
(Hinton, Sutskever, and Krizhevsky)

Human error ~5%

Source: Quartz, [link]()

Neural networks are not appropriate for every problem

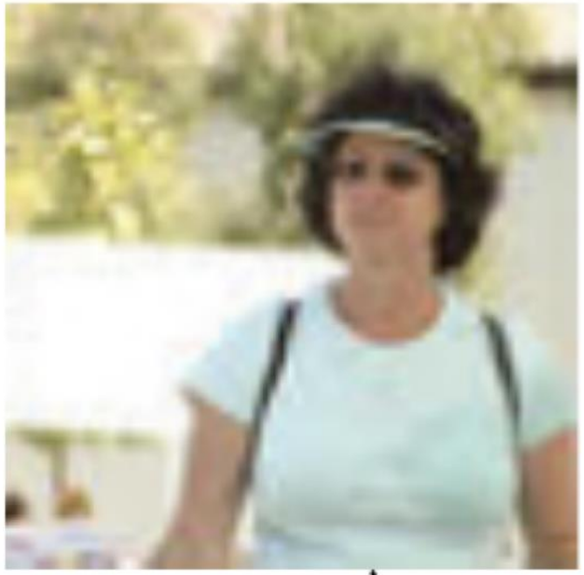
- Small datasets
- Heterogeneous, tabular data
- Cases when model interpretability is paramount

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



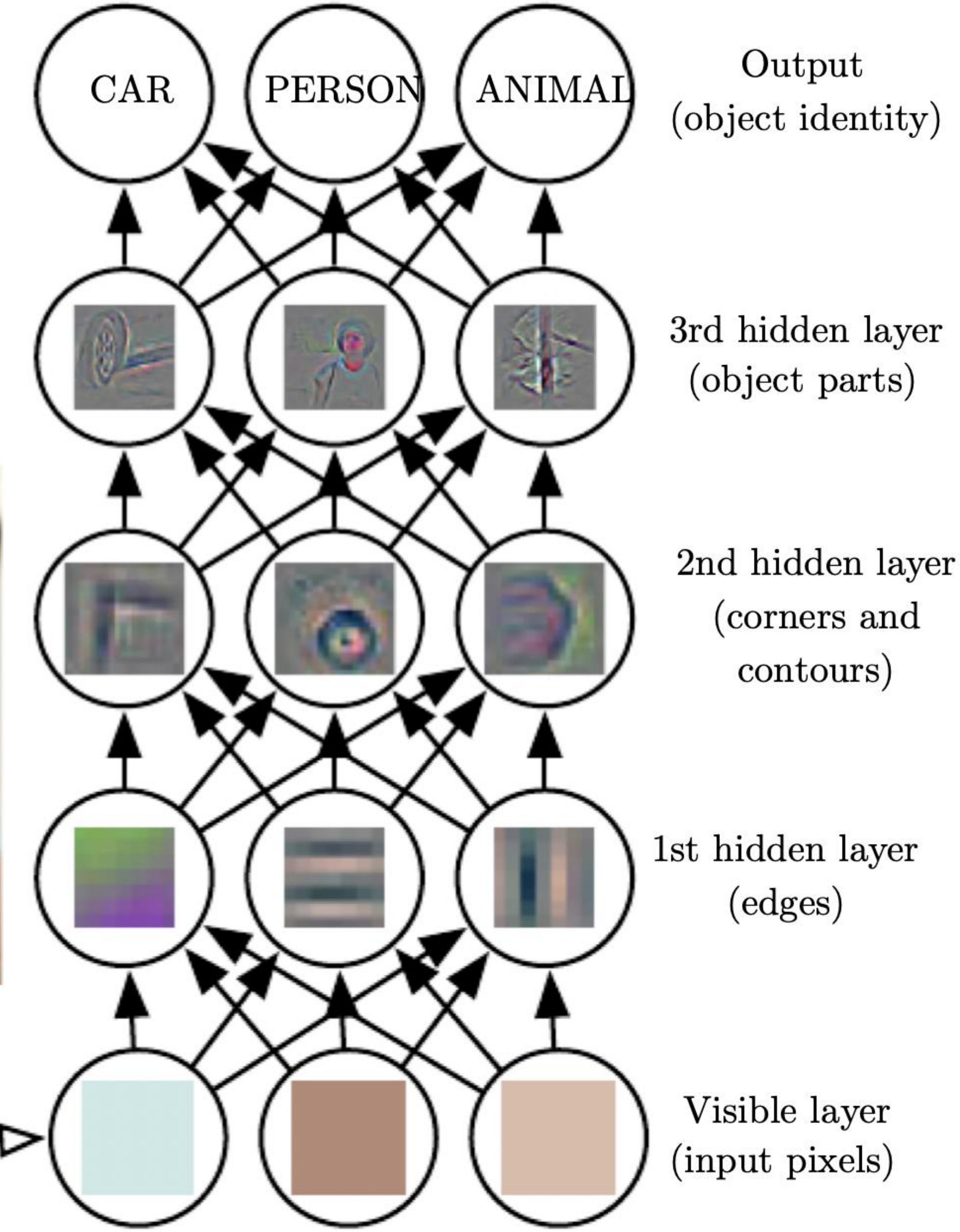
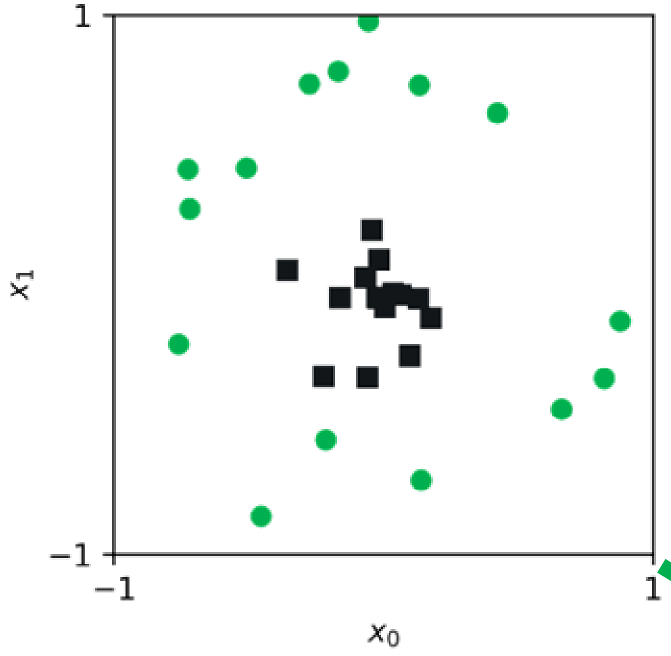


Image from Goodfellow, I., Bengio, Y., Courville, A. and Bengio, Y., 2016. Deep learning (Vol. 1, No. 2). Cambridge: MIT press.

1

Original data

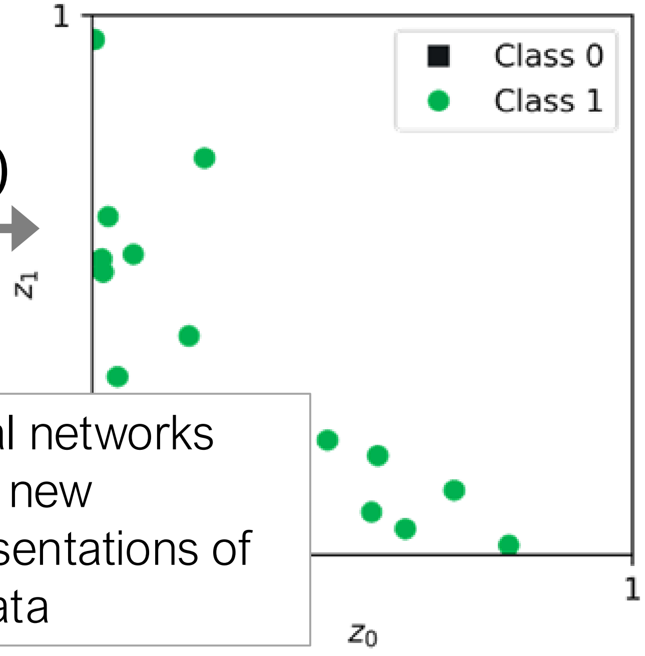
$\boldsymbol{x}$



transform the data

$$\boldsymbol{z} = \Phi(\boldsymbol{x})$$

2



This example transform is quadratic

$$z_i = \Phi(x_i) = x_i^2$$

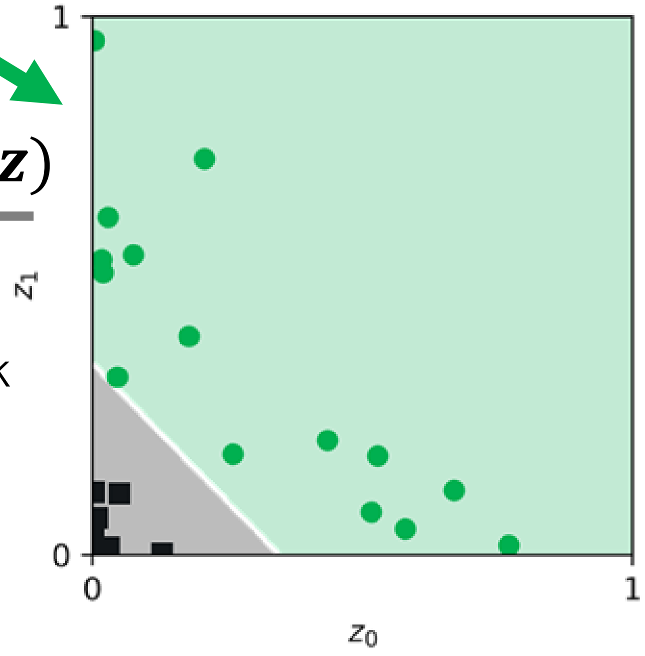
$$z_0 = x_0^2$$

$$z_1 = x_1^2$$

Neural networks **learn** new representations of the data

Classify the features in this Z-space

$$\hat{f}_z(\boldsymbol{z}) = \begin{cases} 1 & \boldsymbol{w}^T\boldsymbol{z} > 0 \\ 0 & else \end{cases}$$



A new **representation** of our data

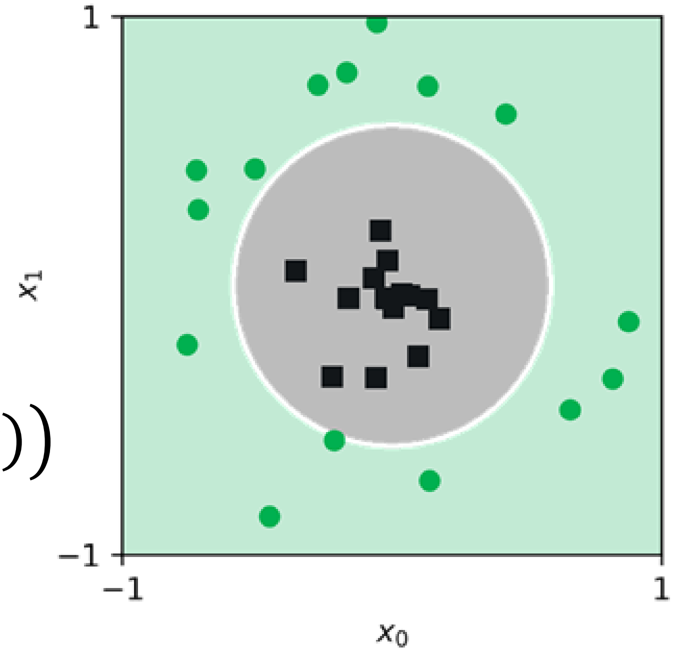
3

$$\boldsymbol{x} = \Phi^{-1}(\boldsymbol{z})$$

transform the data back

$$x_0 = z_0^{1/2}$$

$$x_1 = z_1^{1/2}$$



Predictions in the original X-space

$$\hat{f}(\boldsymbol{x}) = \hat{f}_z(\Phi(\boldsymbol{x}))$$

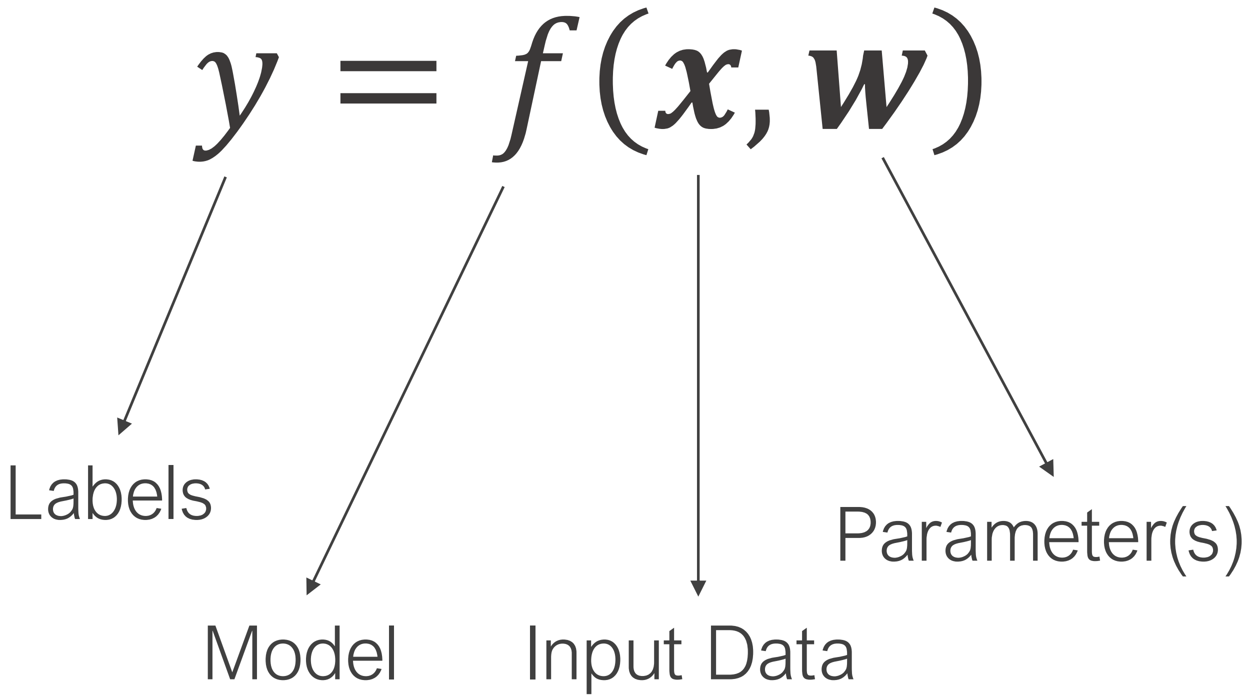
4

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

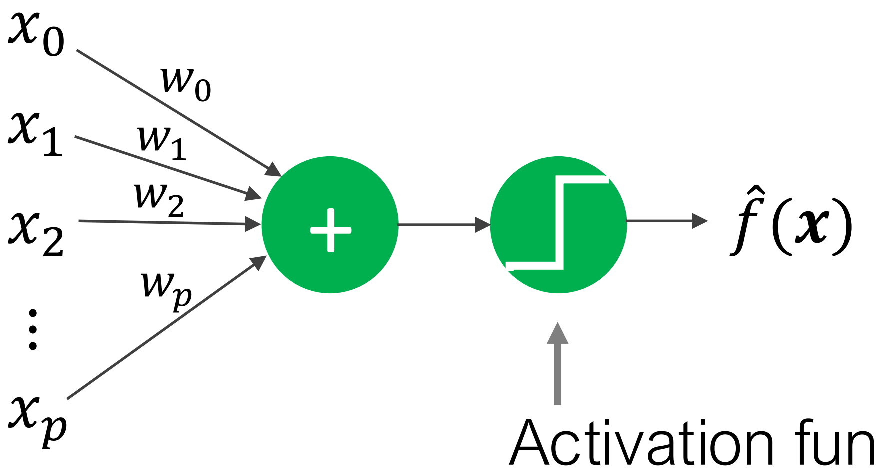
Model

Input Data

Parameter(s)

Perceptron

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

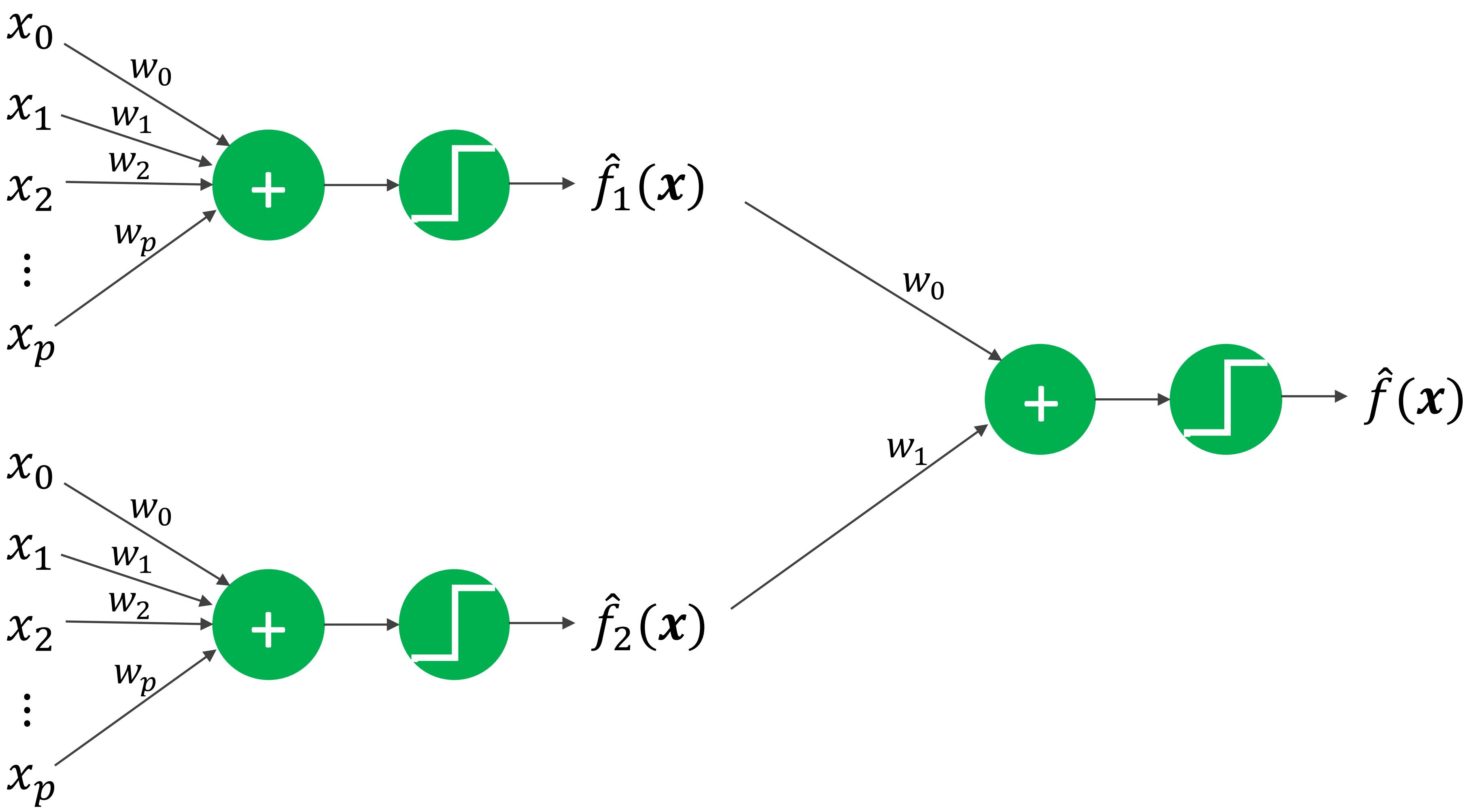


Activation function

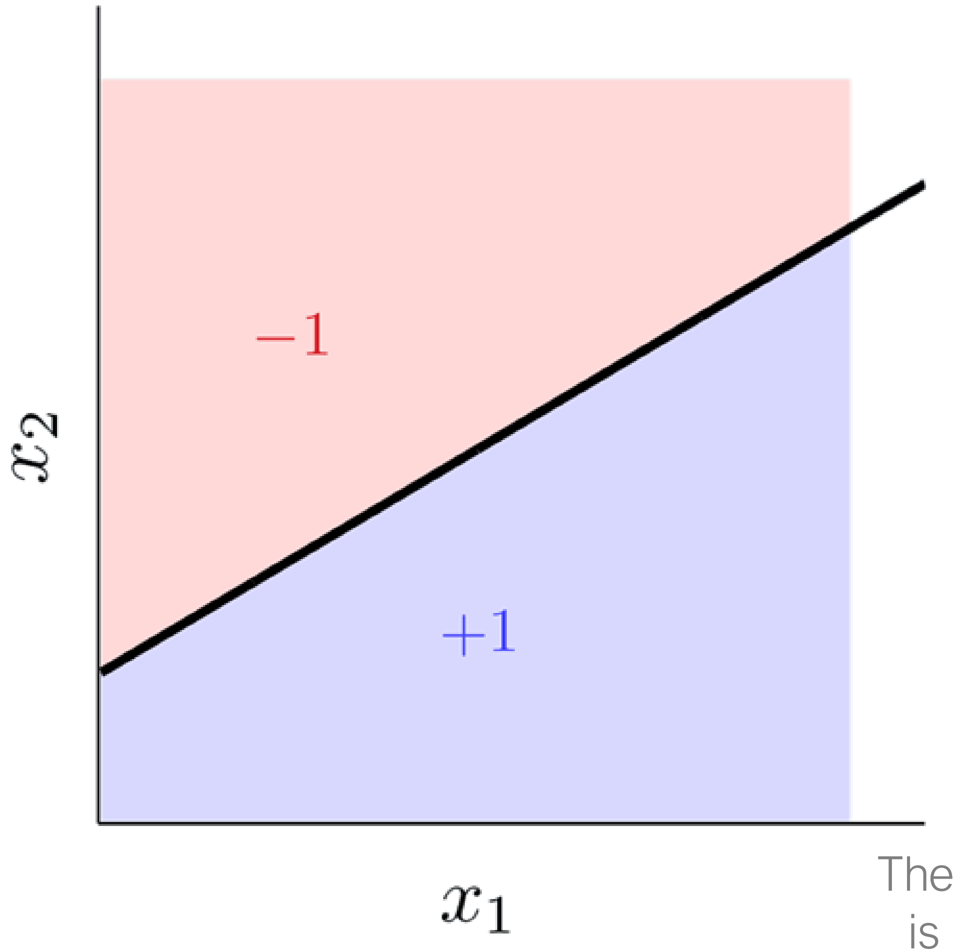
Source: Abu-Mostafa, Learning from Data, Caltech

Multilayer Perceptron

What if we stuck multiple perceptrons together?



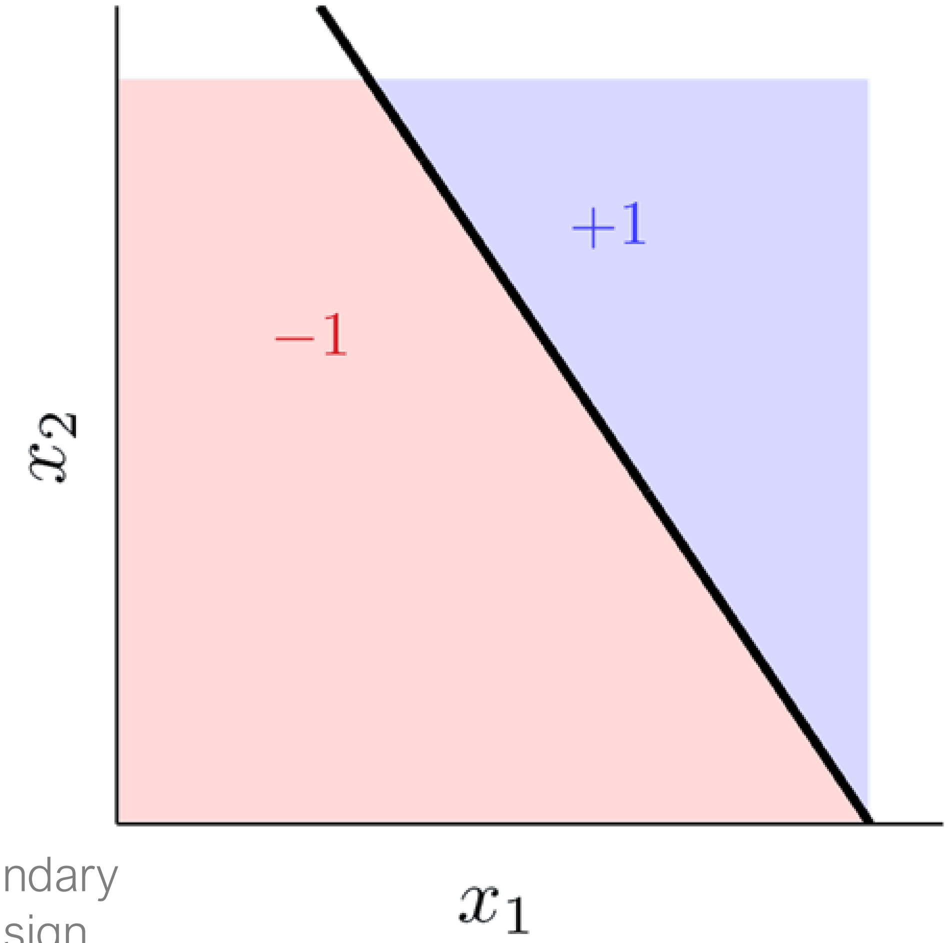
Perceptron #1



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

The sharp boundary is due to our sign function

Perceptron #2

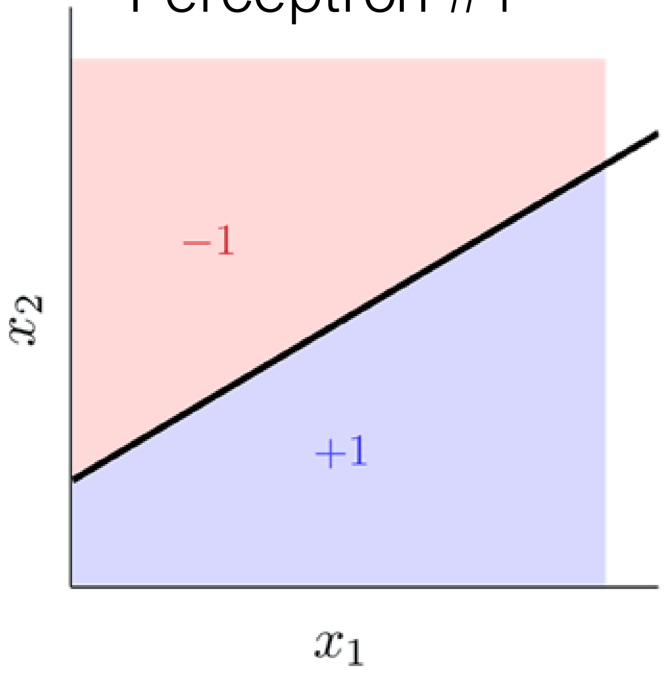


$$\hat{f}_2(\boldsymbol{x}) = sign(\boldsymbol{w}_2^T\boldsymbol{x})$$

Source: Abu-Mostafa, Learning from Data, Caltech

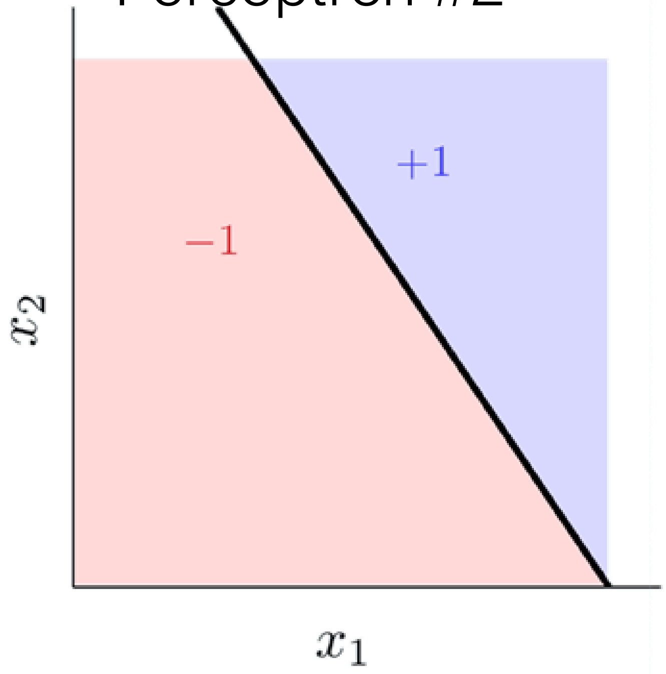
Multilayer perceptron: $\hat{f}(\boldsymbol{x}) = \hat{f}_1(\boldsymbol{x}) - \hat{f}_2(\boldsymbol{x})$

Perceptron #1

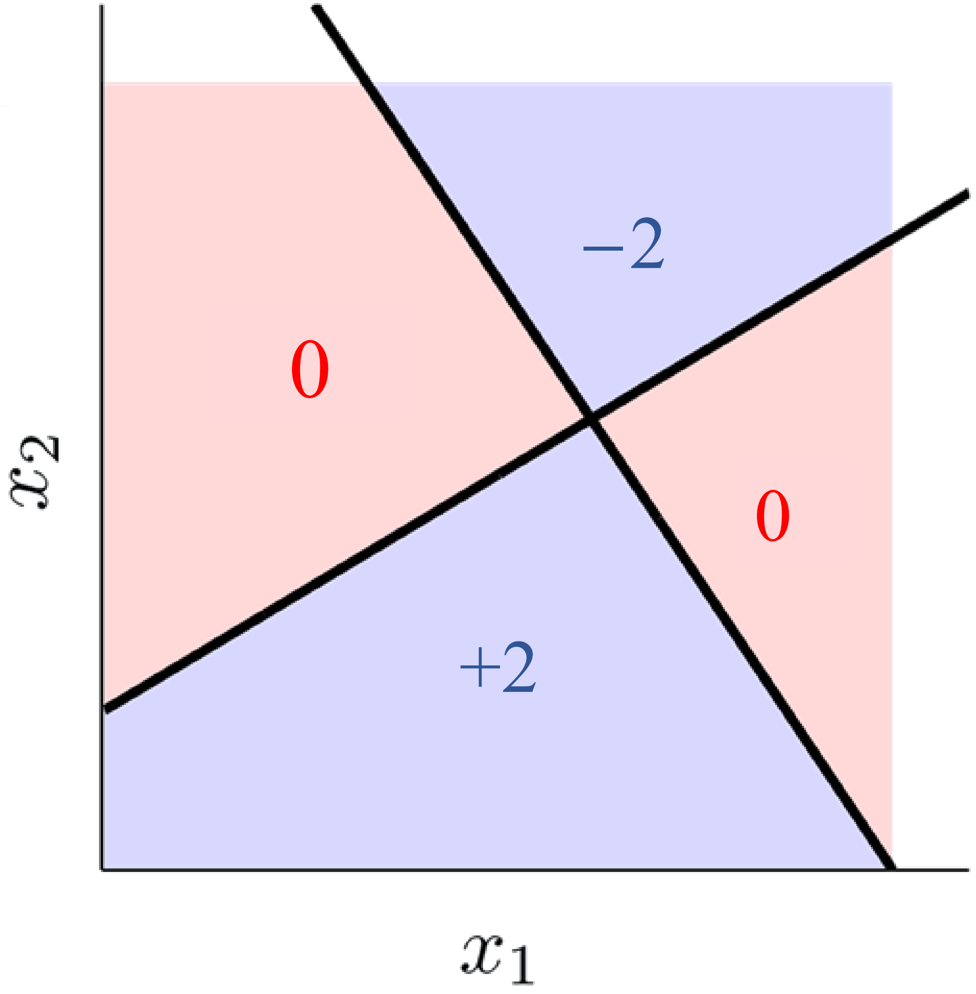


$$\hat{f}_1(\boldsymbol{x}) = sign(\boldsymbol{w}_1^T \boldsymbol{x})$$

Perceptron #2

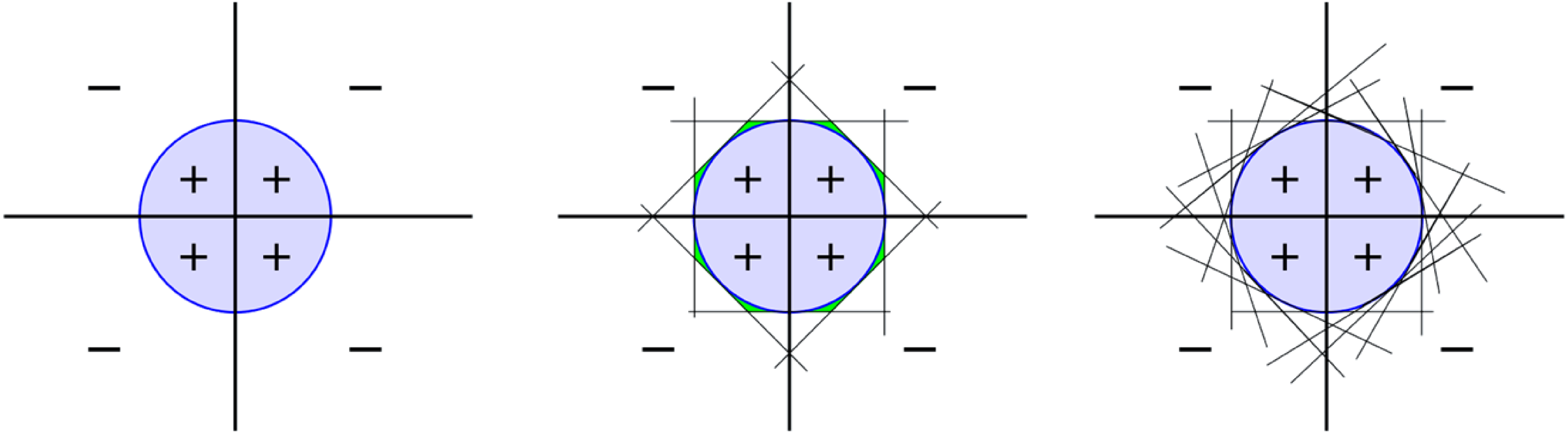


$$\hat{f}_2(\boldsymbol{x}) = sign(\boldsymbol{w}_2^T \boldsymbol{x})$$



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

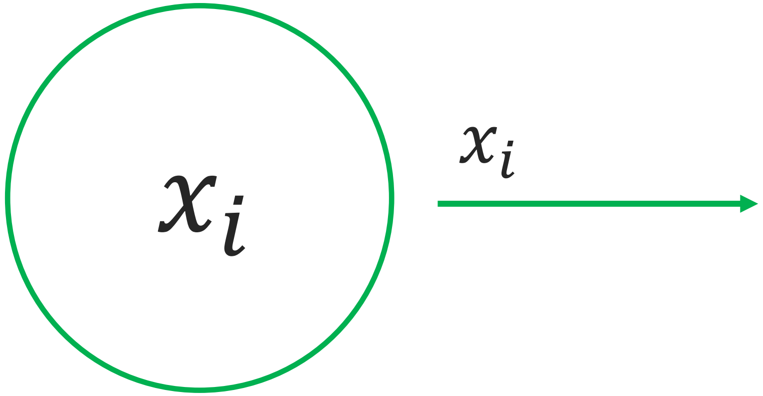
Universal function approximation

"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

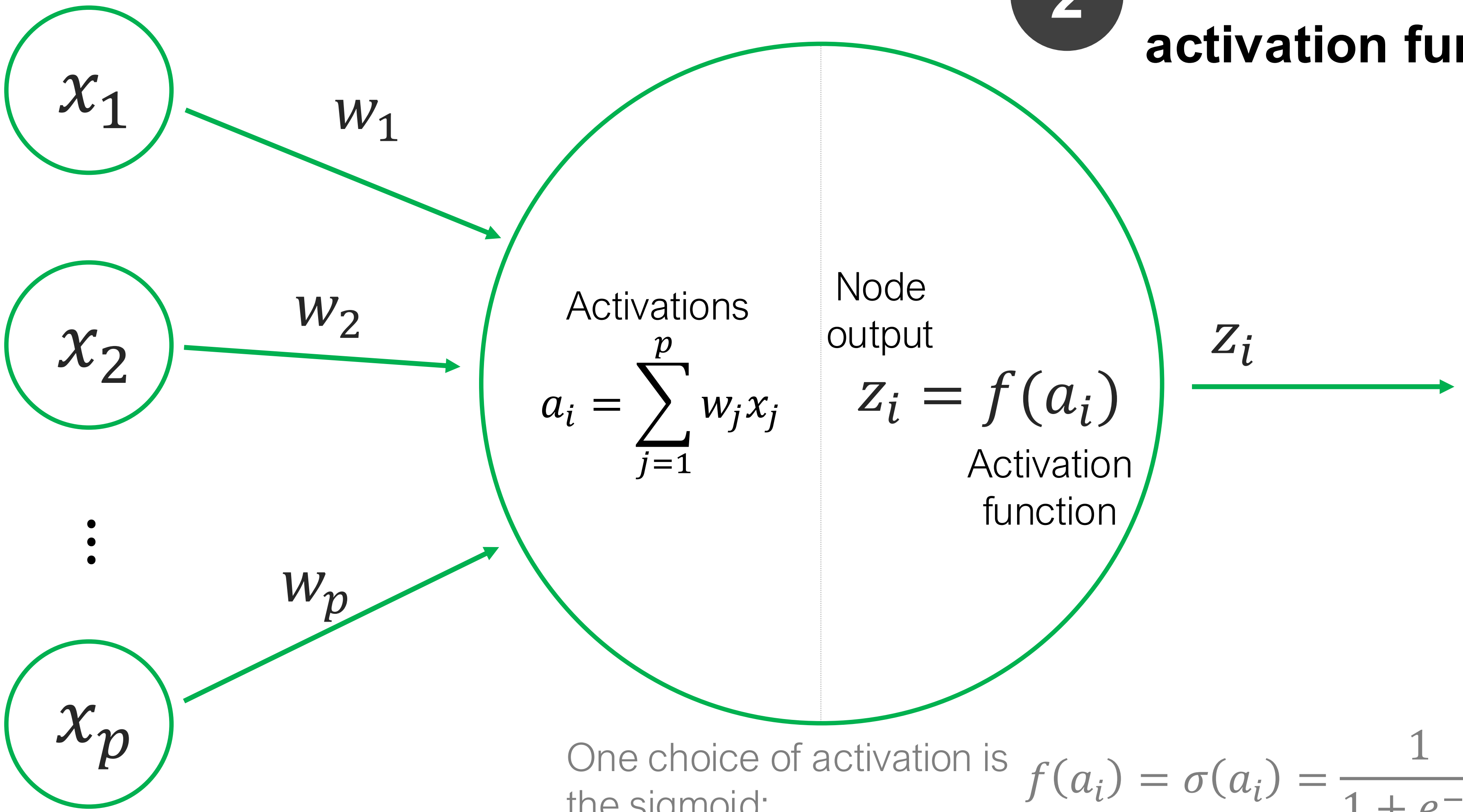
Input nodes / neurons



Simply passes the input value to the next layer

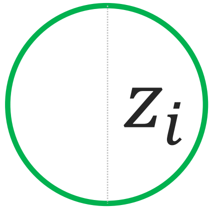
Hidden & output nodes

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

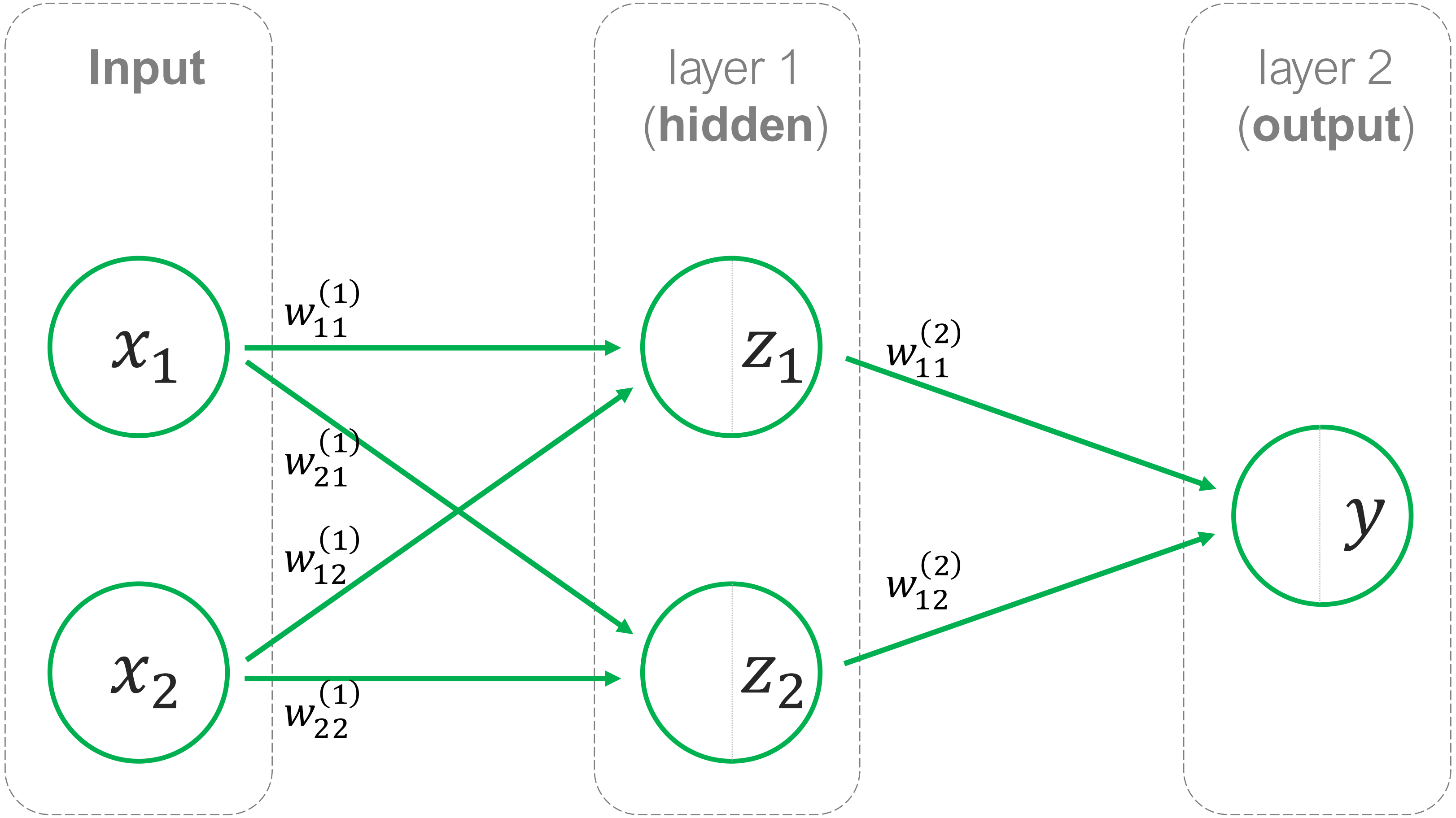


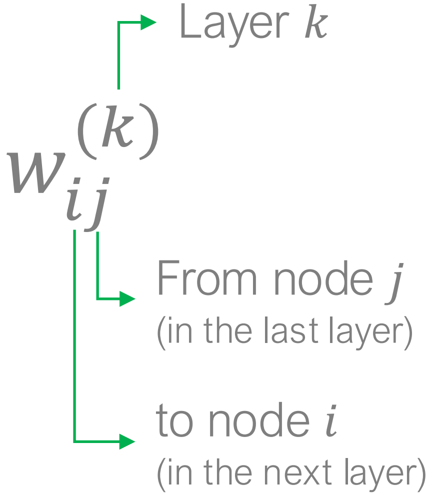
One choice of activation is the sigmoid: $f(a_i) = \sigma(a_i) = \dfrac{1}{1 + e^{-a_i}}$

Represented as:



Simple Neural Network





Layer k

From node j
(in the last layer)

to node i
(in the next layer)

Notational shorthand:
(a more precise
alternative notation)

$z_i = z_i^{(1)}$

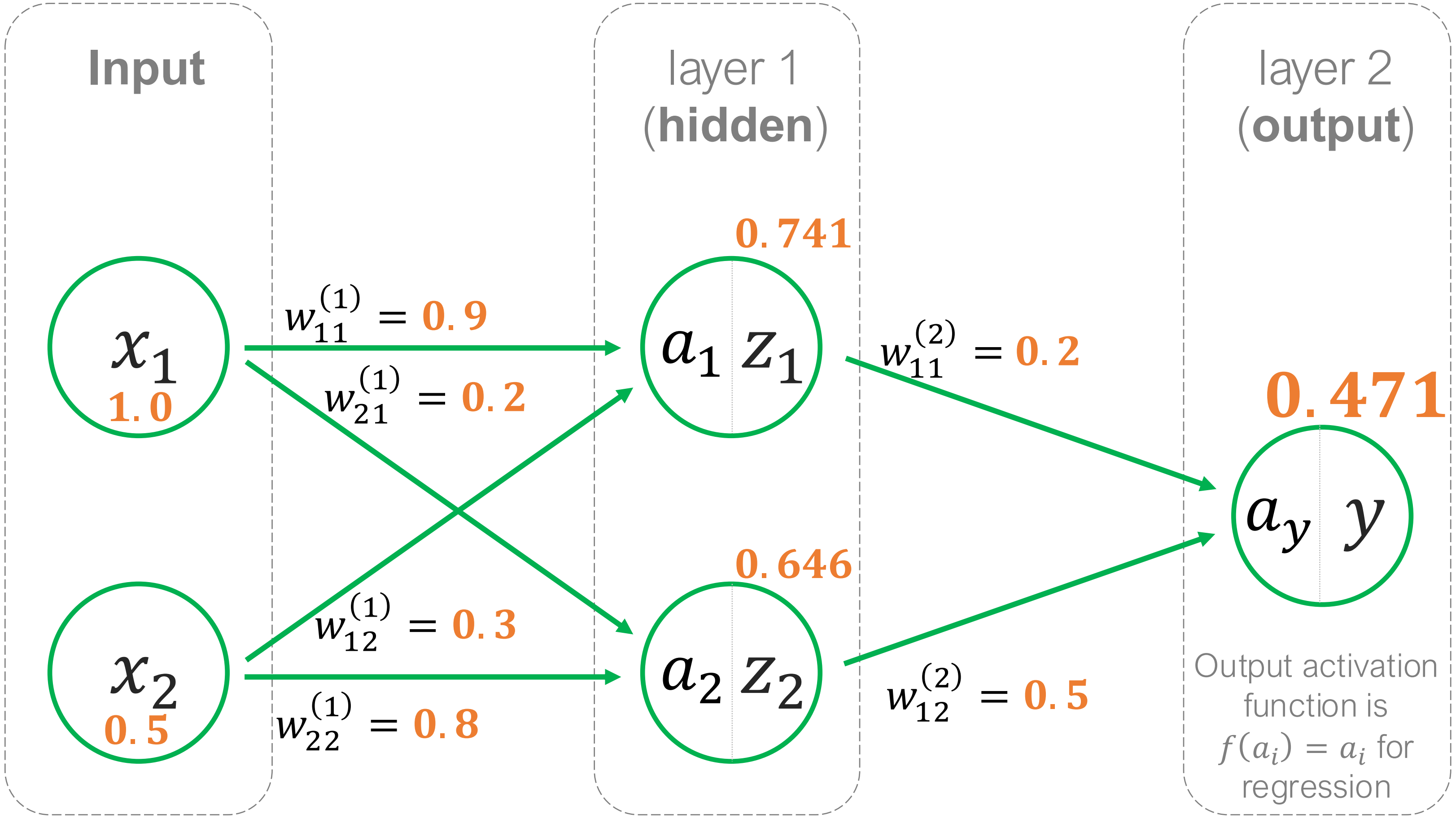
$y = z_1^{(2)}$

Forward Propagation

Calculating the output from input

$$a_1 = (0.9)(1.0) + (0.3)(0.5) = 1.05$$
$$a_2 = (0.2)(1.0) + (0.8)(0.5) = 0.6$$
$$z_1 = \sigma(a_1) = \sigma(1.05) = 0.741$$
$$z_2 = \sigma(a_2) = \sigma(0.6) = 0.646$$

Hidden layer calculations



Output activation function is $f(a_i) = a_i$ for regression

Output layer calculations

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

Regression

Alternatively…

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

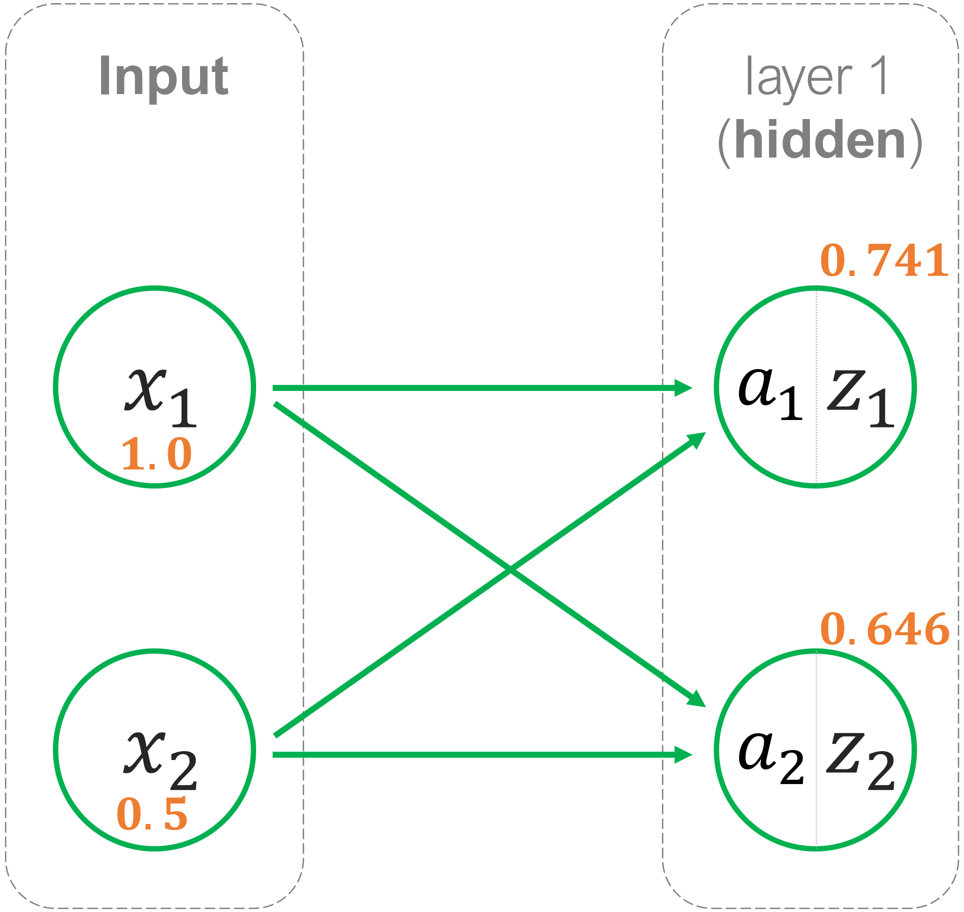
Classification

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

Rashid, Make Your Own Neural Network

Forward Propagation

Calculating the output from input



Hidden layer matrix calculations

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

$$\boldsymbol{W} = \begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{bmatrix} \begin{matrix} \longrightarrow \text{The weights INTO node } z_1 \\ \longrightarrow \text{The weights INTO node } z_2 \end{matrix}$$

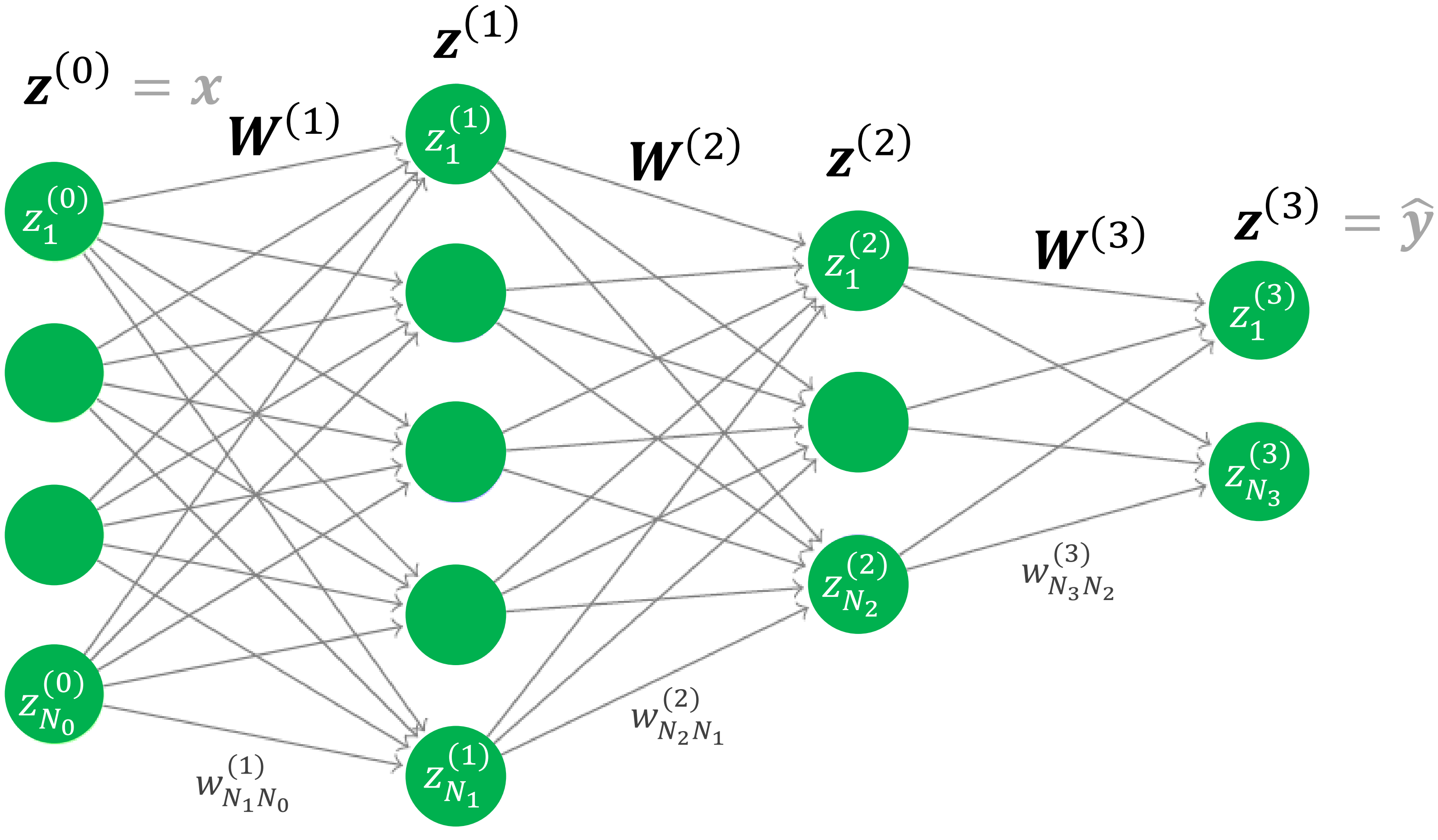
$$\boldsymbol{a} = \boldsymbol{W}\boldsymbol{x} = \begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

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

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

Forward Propagation

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



Sudeep Raja, A Derivation of Backpropagation in Matrix Form

Simple steps for forward propagation:

```
For $i = 1$ to $L$:
    $\boldsymbol{z}^{(i)} = \sigma\left(\boldsymbol{W}^{(i)}\boldsymbol{z}^{(i-1)}\right)$
```

Where:

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

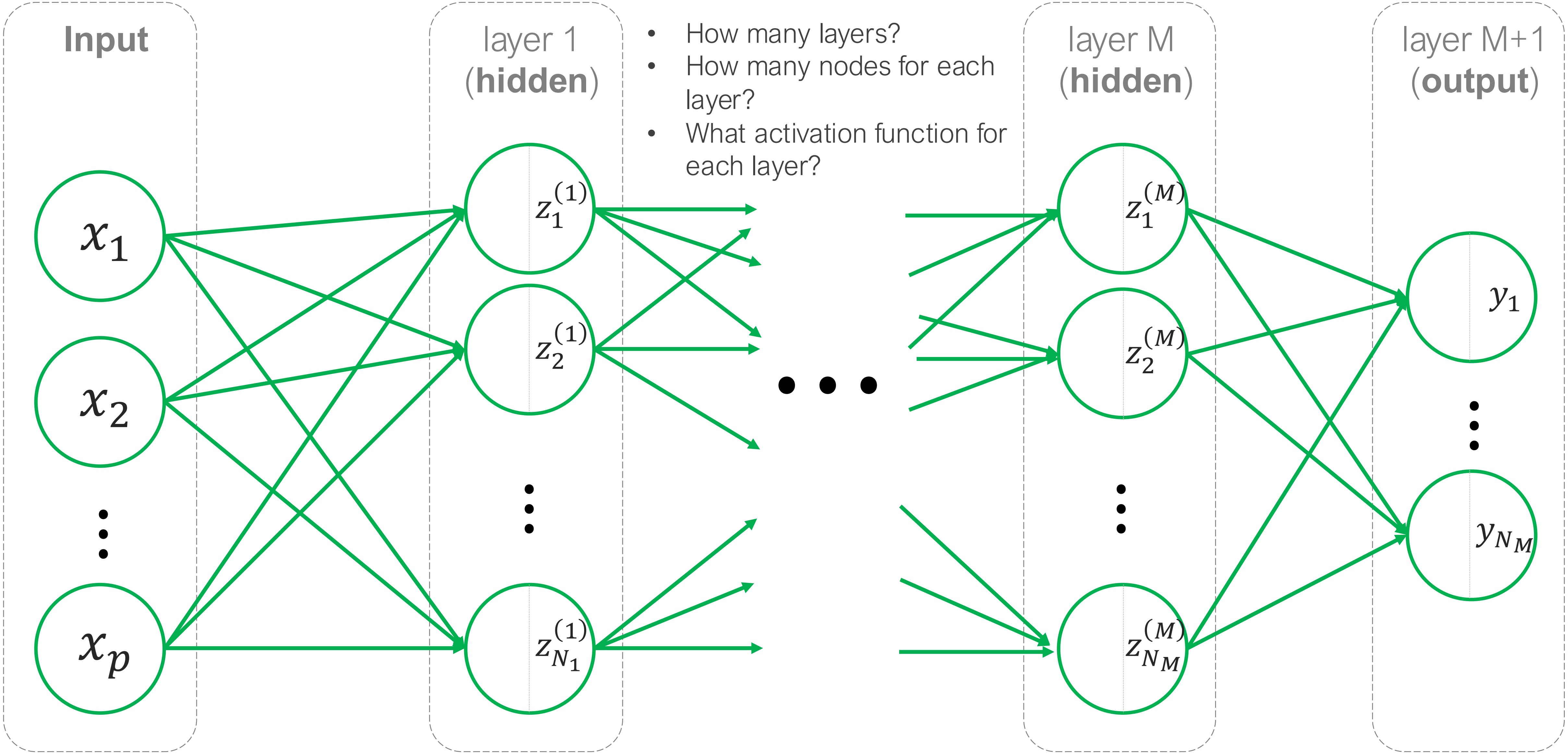
$$\hat{\boldsymbol{y}} = \boldsymbol{z}^{(L)}$$

Prediction error is measured:

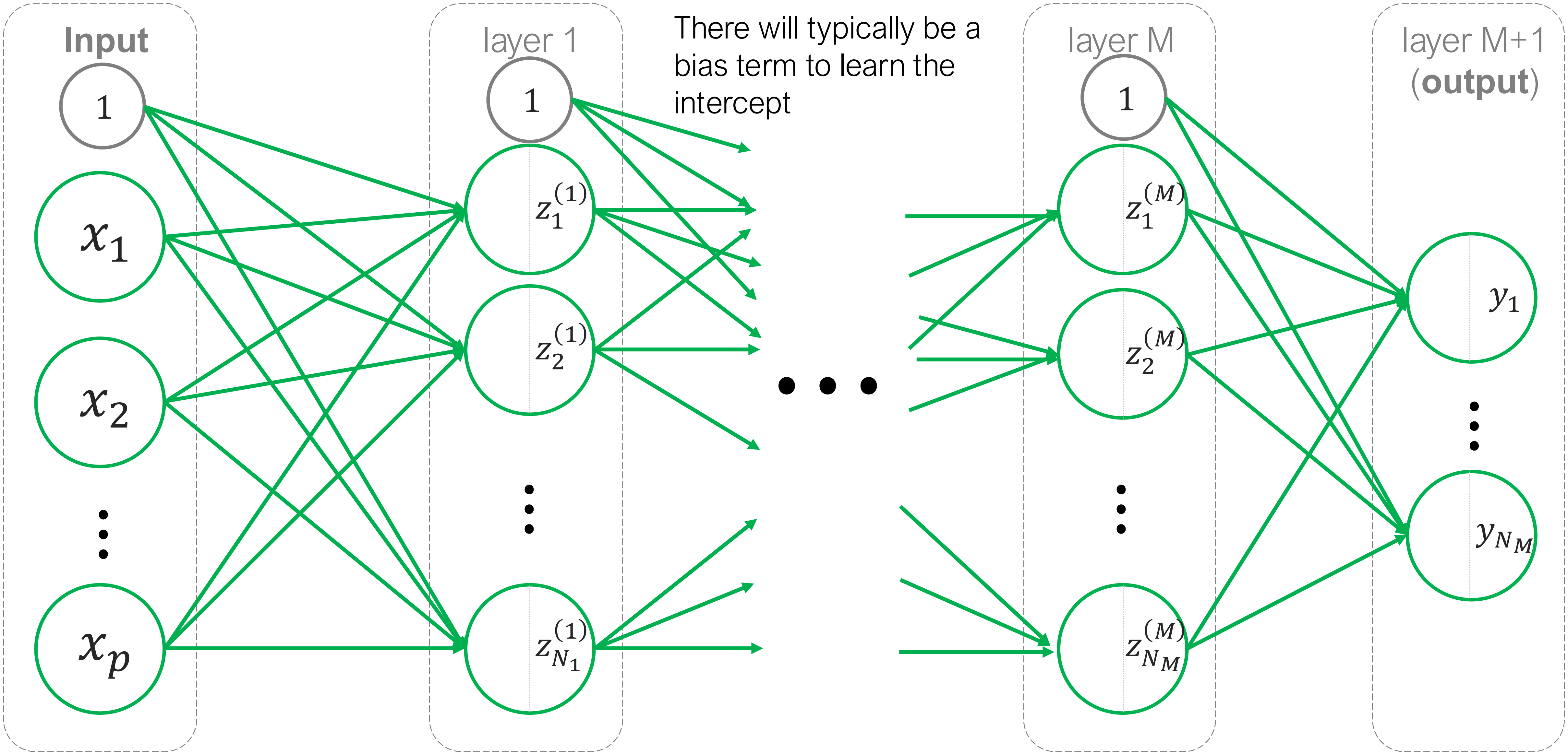
$$E_n = \frac{1}{2}(\hat{y}_n - y_n)^2$$

Neural networks can be customized

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

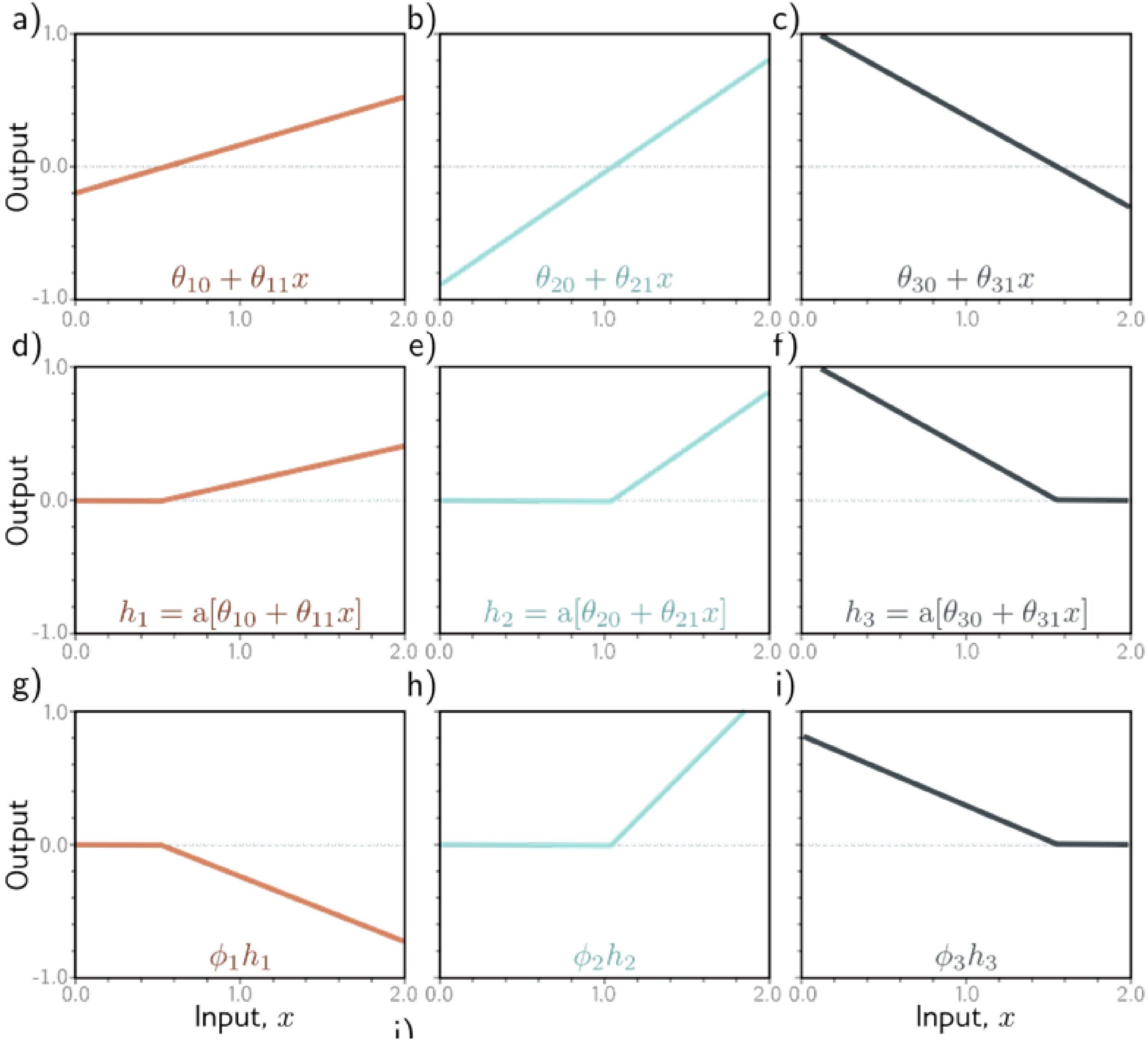


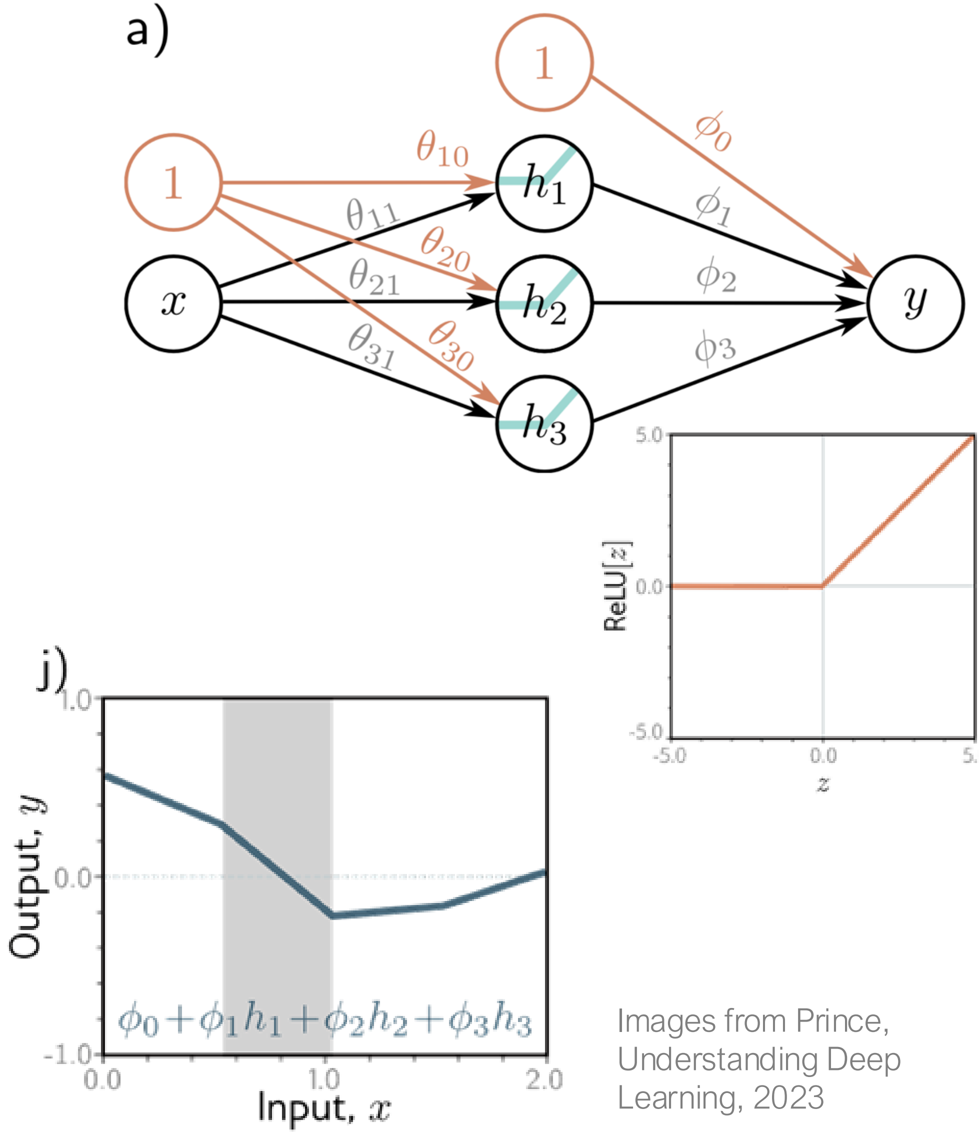
Neural networks can be customized



There will typically be a bias term to learn the intercept

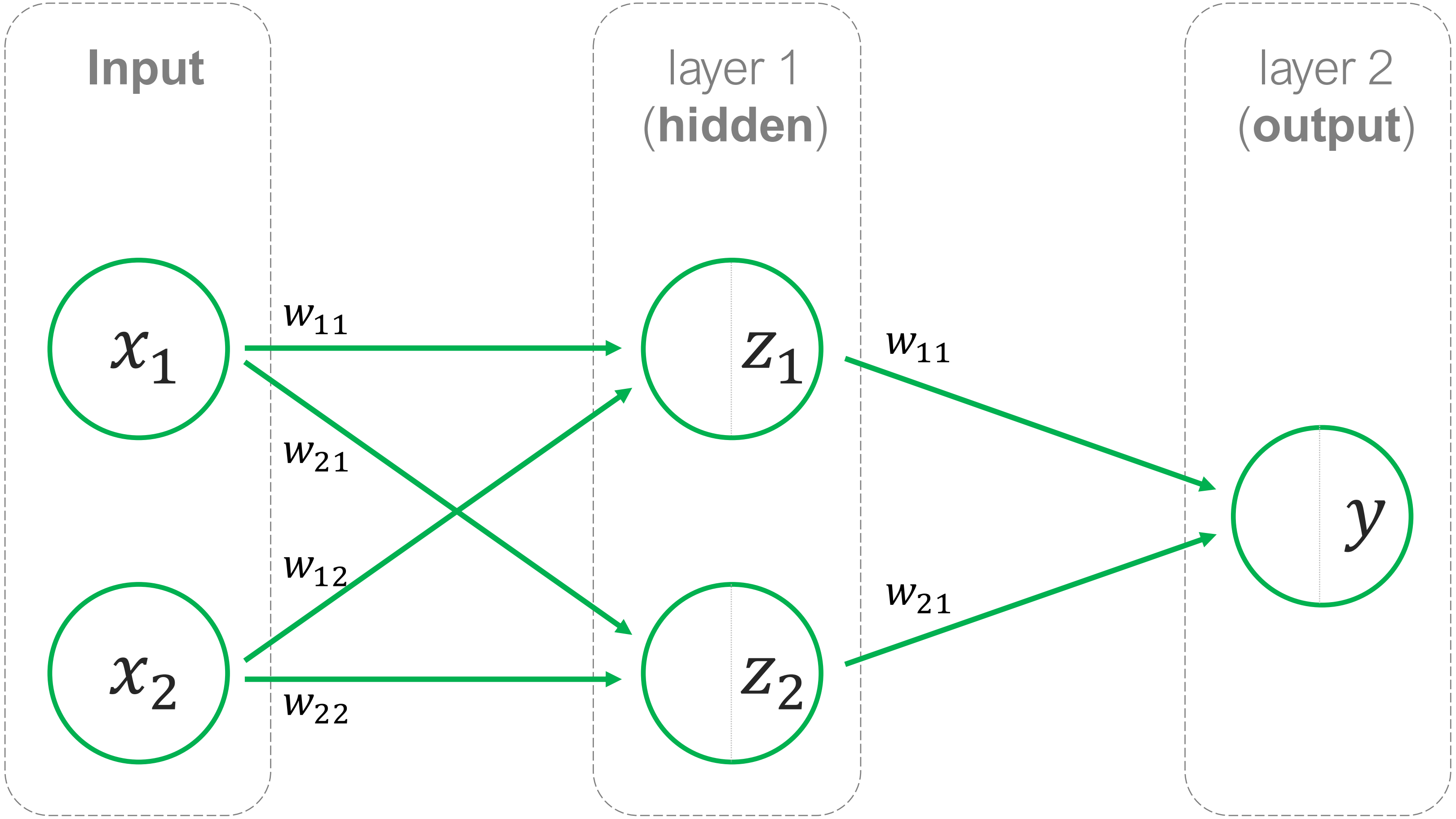
Example of simple neural network for regression





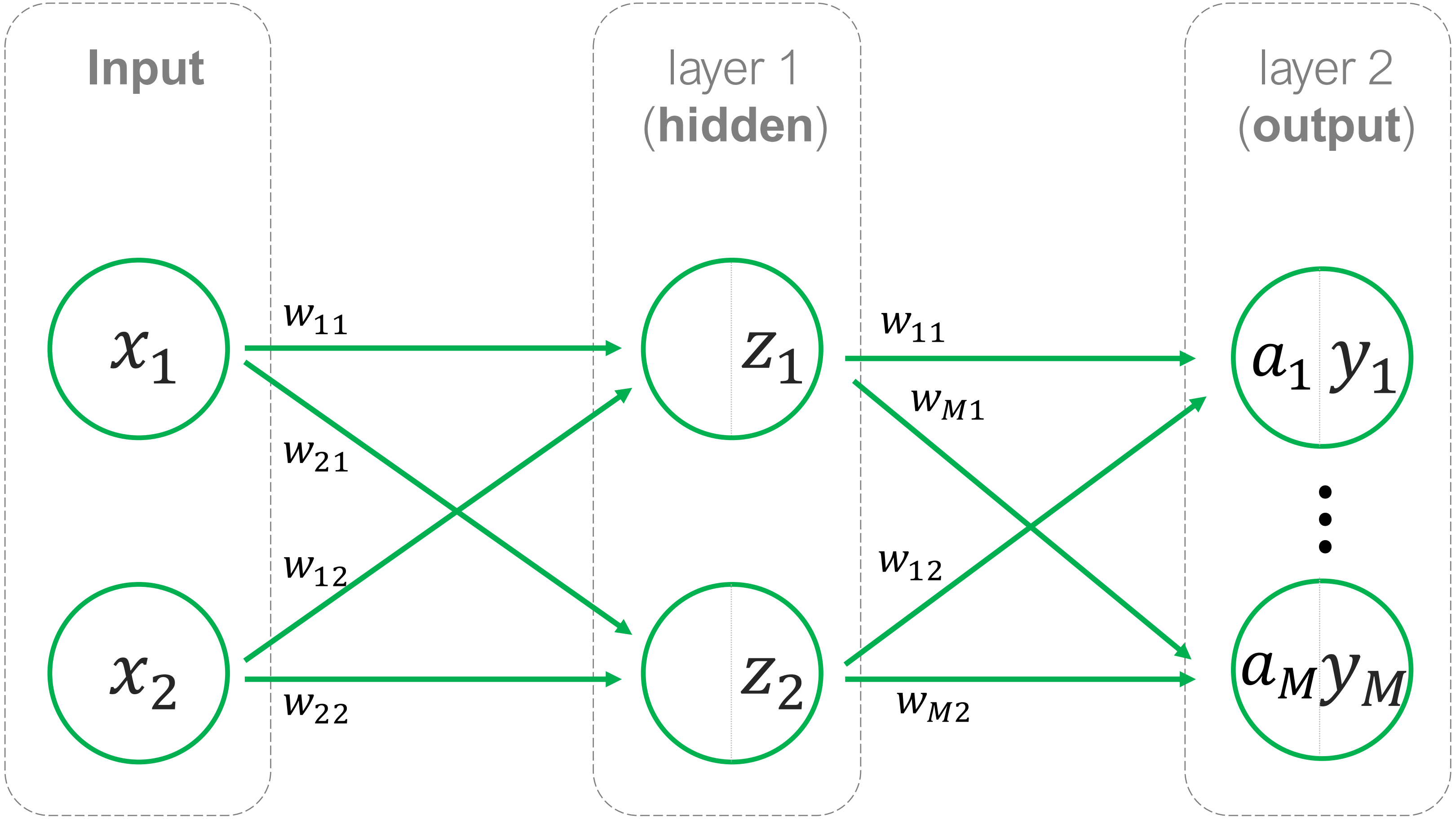
Images from Prince, Understanding Deep Learning, 2023

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)

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

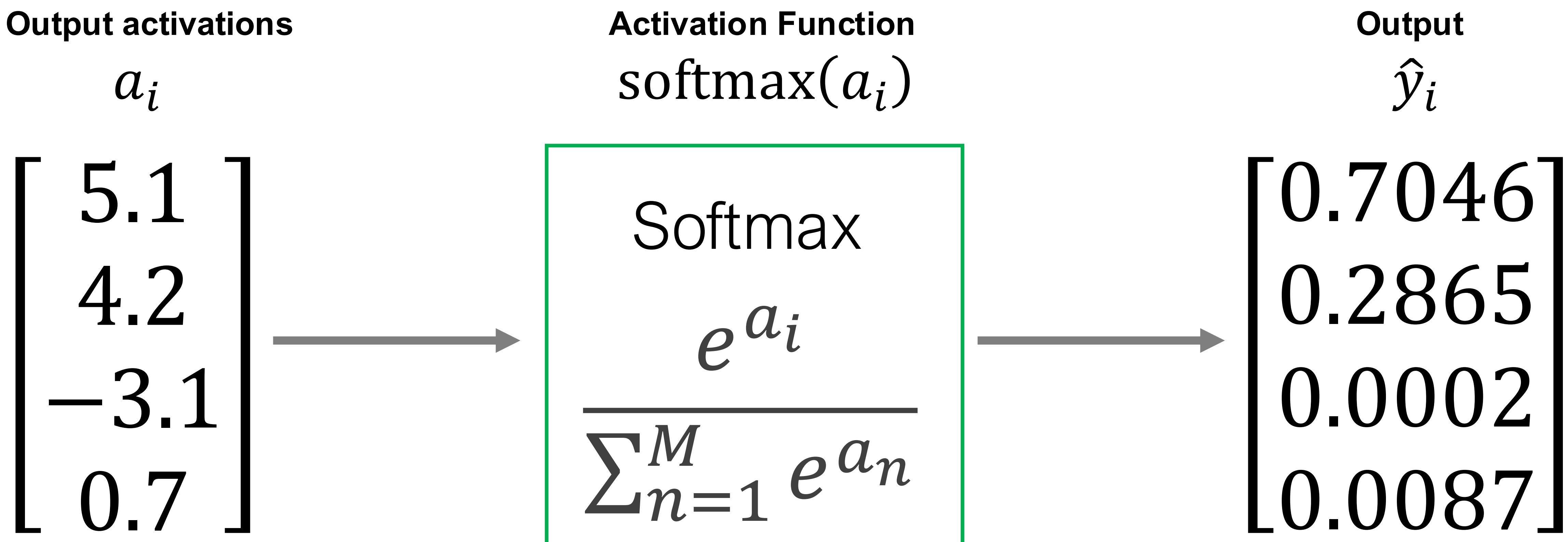
Choose the largest y value as the predicted class

Softmax

Generalization of the logistic function to multiple dimensions

To use softmax as a cost function, we use a similar expression to cross entropy loss:

$$C = -\sum_{i=1}^{M} y_{\mathrm{i}} \log\left(\mathrm{softmax}(a_i)\right)$$



Output activations

a_i

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

Activation Function

$\mathrm{softmax}(a_i)$

Softmax

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

Output

$\hat{y}_i$

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

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?