imprs·mic

Introduction to Neural Networks

Dr. Manuel Gehl

MAX PLANCK INSTITUTE
FOR TERRESTRIAL MICROBIOLOGY

Overview

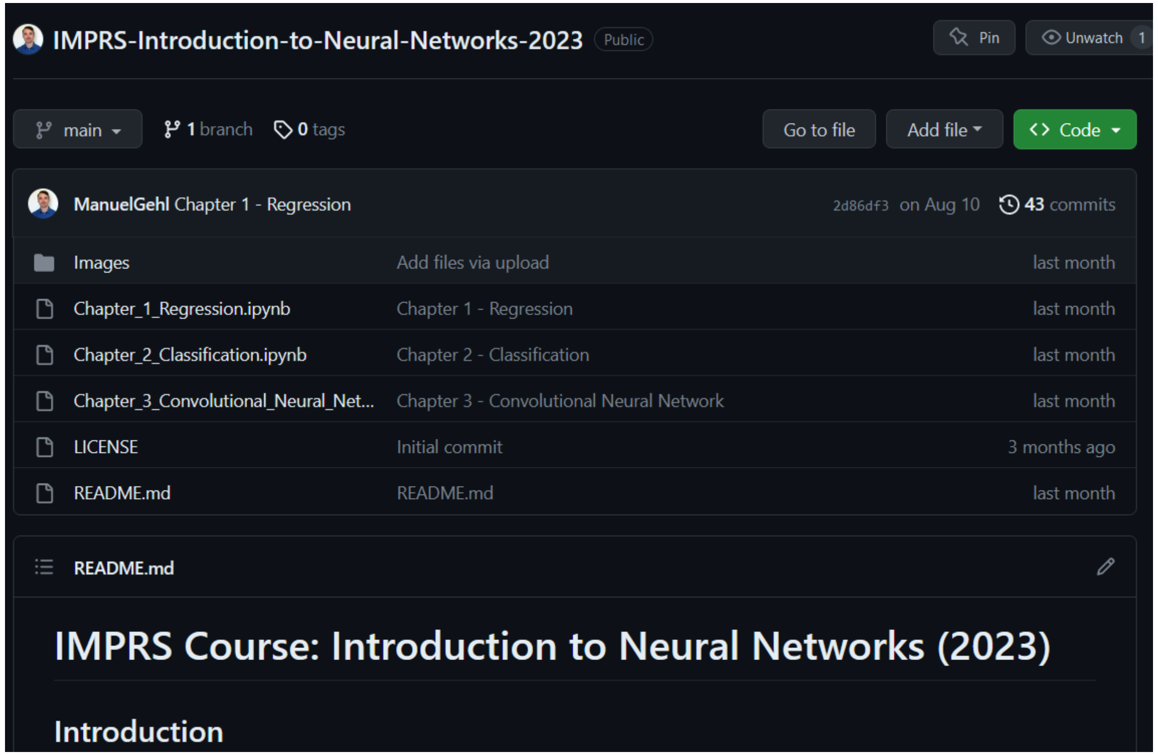
Lecture

- What are Artificial Neural Networks?
- What is an Artificial Neuron?
- How Do Artificial Neurons Learn?
- What next?

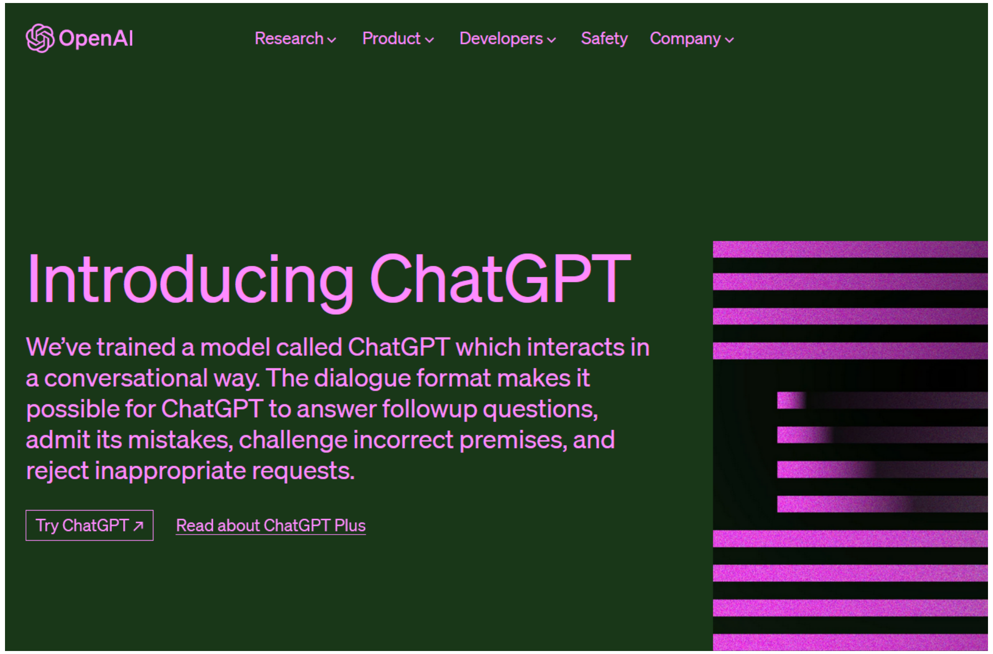
Notebooks

- Chapter 1 – Regression
- Chapter 2 – Classification
- Chapter 3 – Convolutional Neural Networks

Course Website

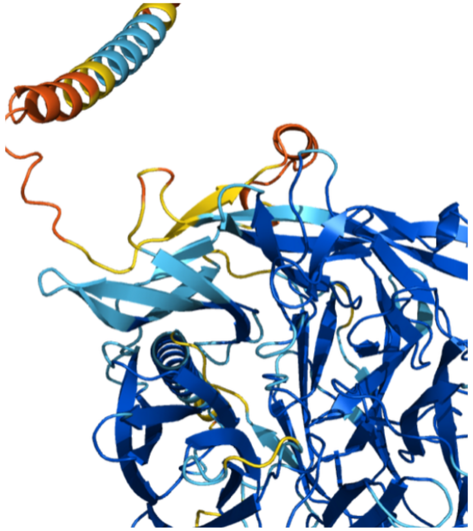


What are Artificial Neural Networks?

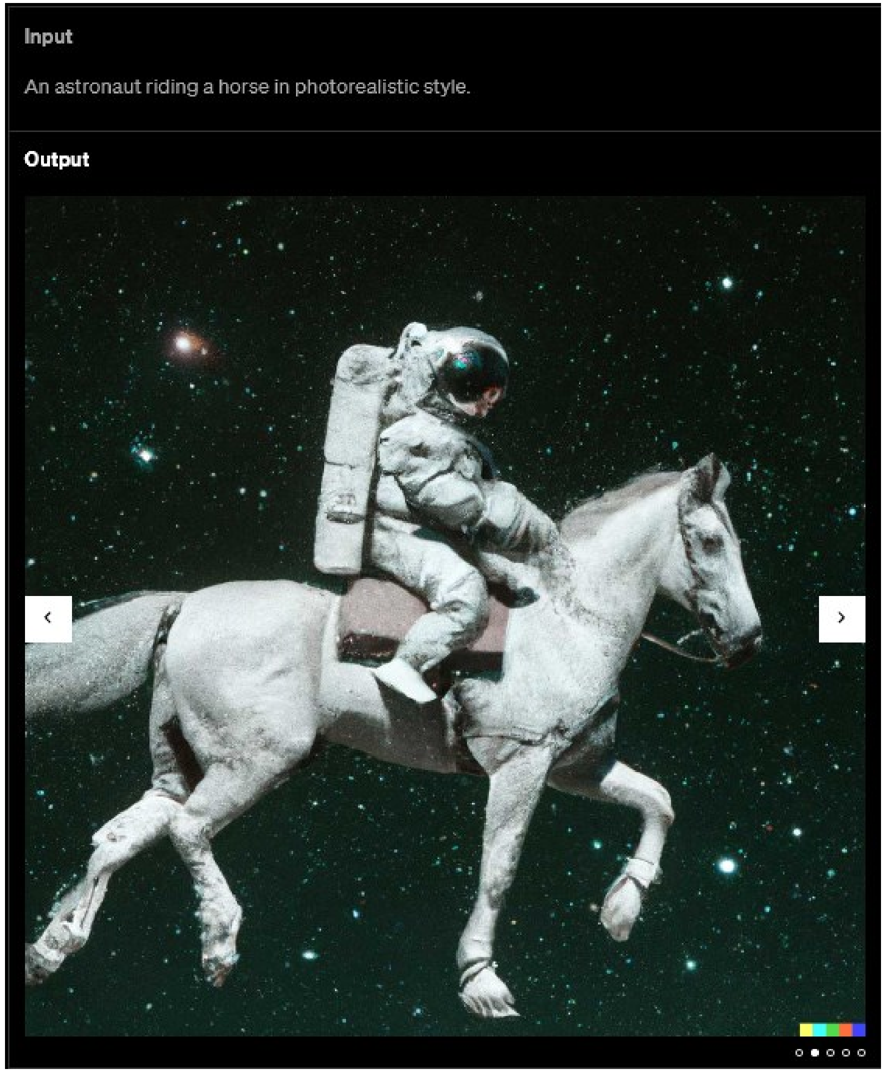


AlphaFold is an AI system developed by DeepMind that predicts a protein's 3D structure from its amino acid sequence. It regularly achieves accuracy competitive with experiment.

DeepMind and EMBL's European Bioinformatics Institute (EMBL-EBI) have partnered to create AlphaFold DB to make these predictions freely available to the scientific community. The latest database release contains over 200 million entries, providing broad coverage of UniProt (the standard repository of protein sequences and annotations). We provide individual downloads for the human proteome and for the proteomes of 47 other key organisms important in research and global health. We also provide a download for the manually curated subset of UniProt (Swiss-Prot).



Q8I3H7: May protect the malaria parasite against attack by the immune system.
Mean pLDDT 85.57.



What are Artificial Neural Networks?

Deep Learning for Protein–Protein Interaction Site Prediction

Arian R. Jamasb, Ben Day, Cătălina Cangea, Pietro Liò & Tom L. Blundell

Protocol | Open Access | First Online: 09 July 2021

Part of the Methods in Molecular Biology book series (MIMB,volume 2361)

De novo design of luciferases using deep learning

Andy Hsien-Wei Yeh, Christoffer Norn, Yakov Kipnis, Doug Tischer, Samuel J. Pellock, Declan Evans, Pengchen Ma, Gyu Rie Lee, Jason Z. Zhang, Ivan Anishchenko, Brian Coventry, Longxing Cao, Justas Dauparas, Samer Halabiya, Michelle DeWitt, Lauren Carter, K. N. Houk & David Baker

Nature **614**, 774–780 (2023) | Cite this article

Classification and mutation prediction from non–small cell lung cancer histopathology images using deep learning

Nicolas Coudray, Paolo Santiago Ocampo, Theodore Sakellaropoulos, Navneet Narula, Matija Snuderl, David Fenyö, Andre L. Moreira, Narges Razavian & Aristotelis Tsirigos

Nature Medicine **24**, 1559–1567 (2018) | Cite this article

Geometric deep learning of RNA structure

RAPHAEL J. L. TOWNSHEND, STEPHAN EISMANN, ANDREW M. WATKINS, RAMYA RANGAN, MASHA KARELINA, RHIJU DAS, AND RON O. DROR

Authors Info & Affiliations

SCIENCE • 26 Aug 2021 • Vol 373, Issue 6558 • pp. 1047-1051 • DOI: 10.1126/science.abe5650

Scaffolding protein functional sites using deep learning

JUE WANG, SIDNEY LISANZA, DAVID JUERGENS, DOUG TISCHER, JOSEPH L. WATSON, KARLA M. CASTRO, ROBERT RAGOTTE, AMIJAI SARAGOVI, LUKAS F. MILLES, [...], AND DAVID BAKER +14 authors Authors Info & Affiliations

SCIENCE • 21 Jul 2022 • Vol 377, Issue 6604 • pp. 387-394 • DOI: 10.1126/science.abn2100

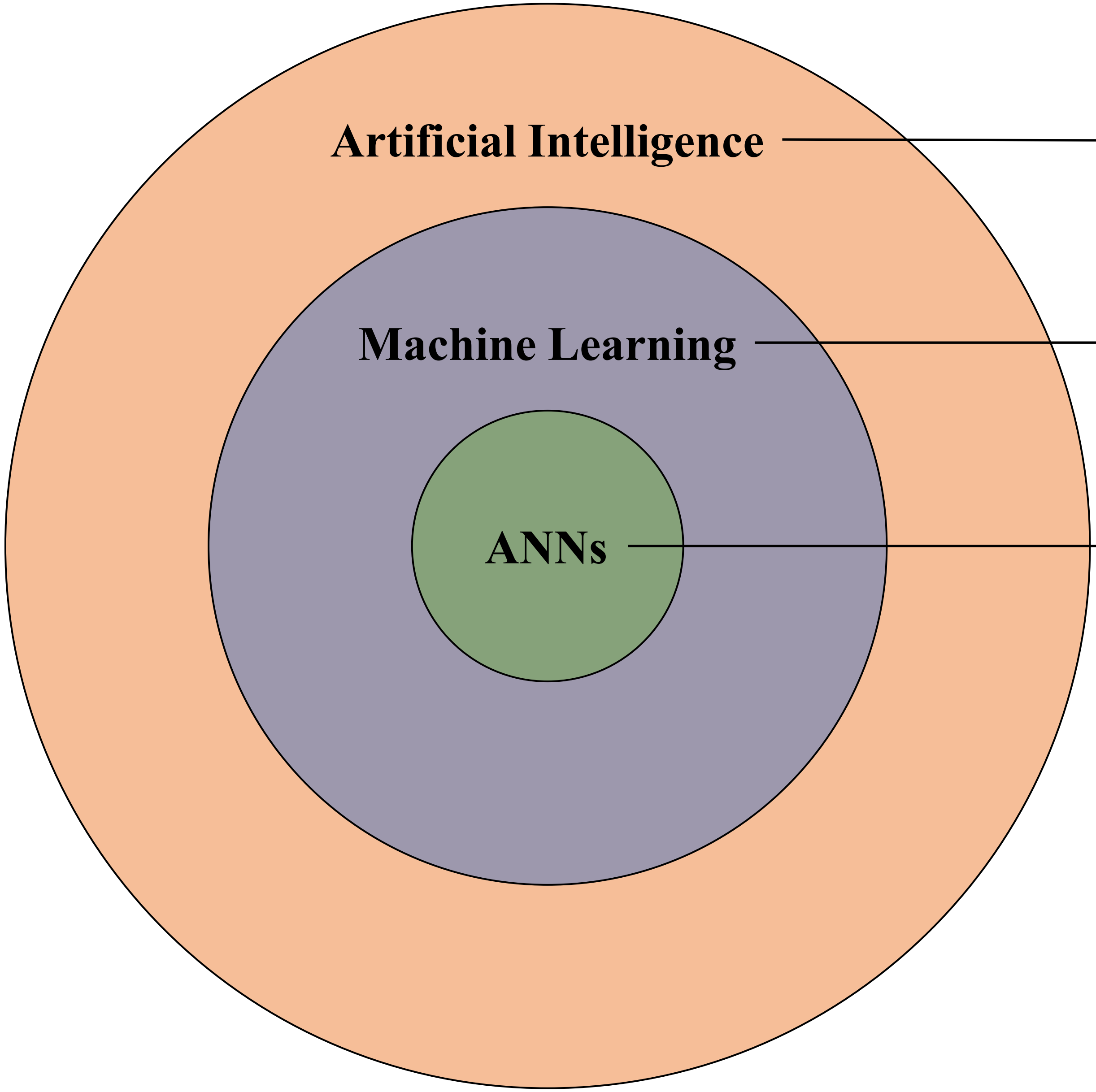
STRUCTURAL BIOLOGY

Protein sequence design by deep learning

Jue Wang

Nature Computational Science **2**, 416–417 (2022) | Cite this article

What are Artificial Neural Networks?



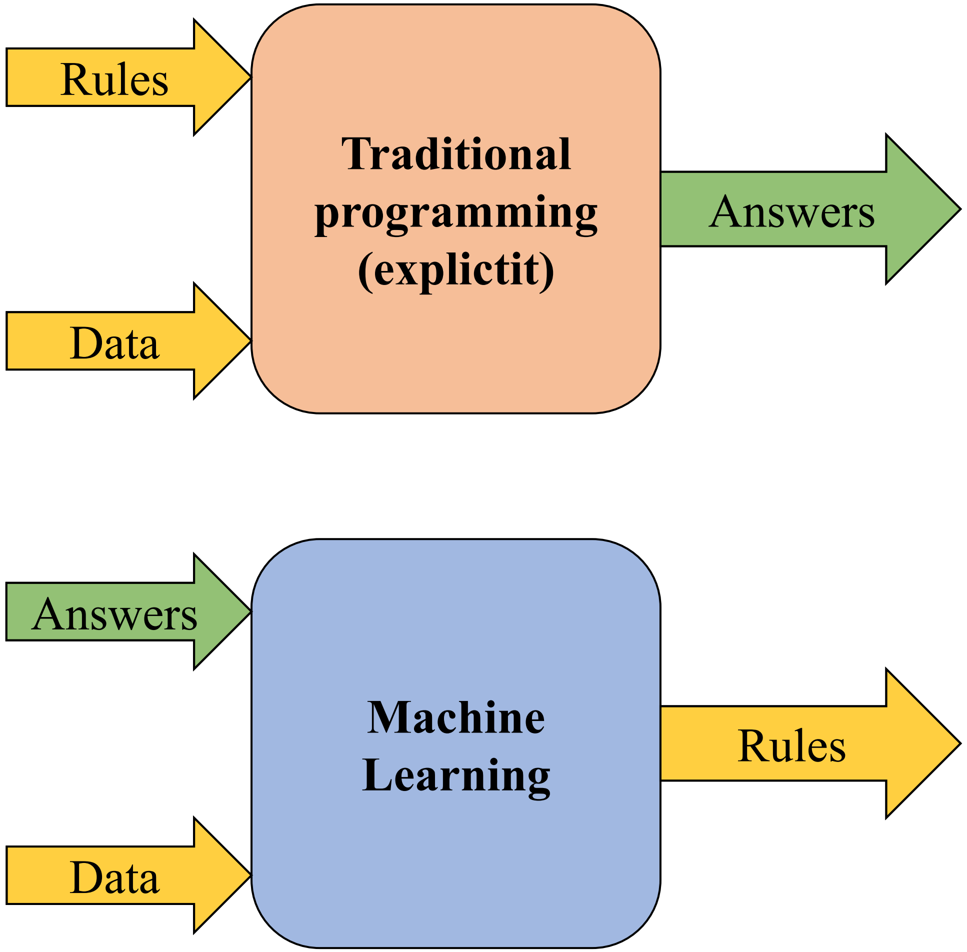
AI = Techniques that allow computers to mimic the behavior of human beings

ML = Technique that allows a machine to learn without being explicitly programmed

ANN = ML technique based on the architecture of biological neural networks

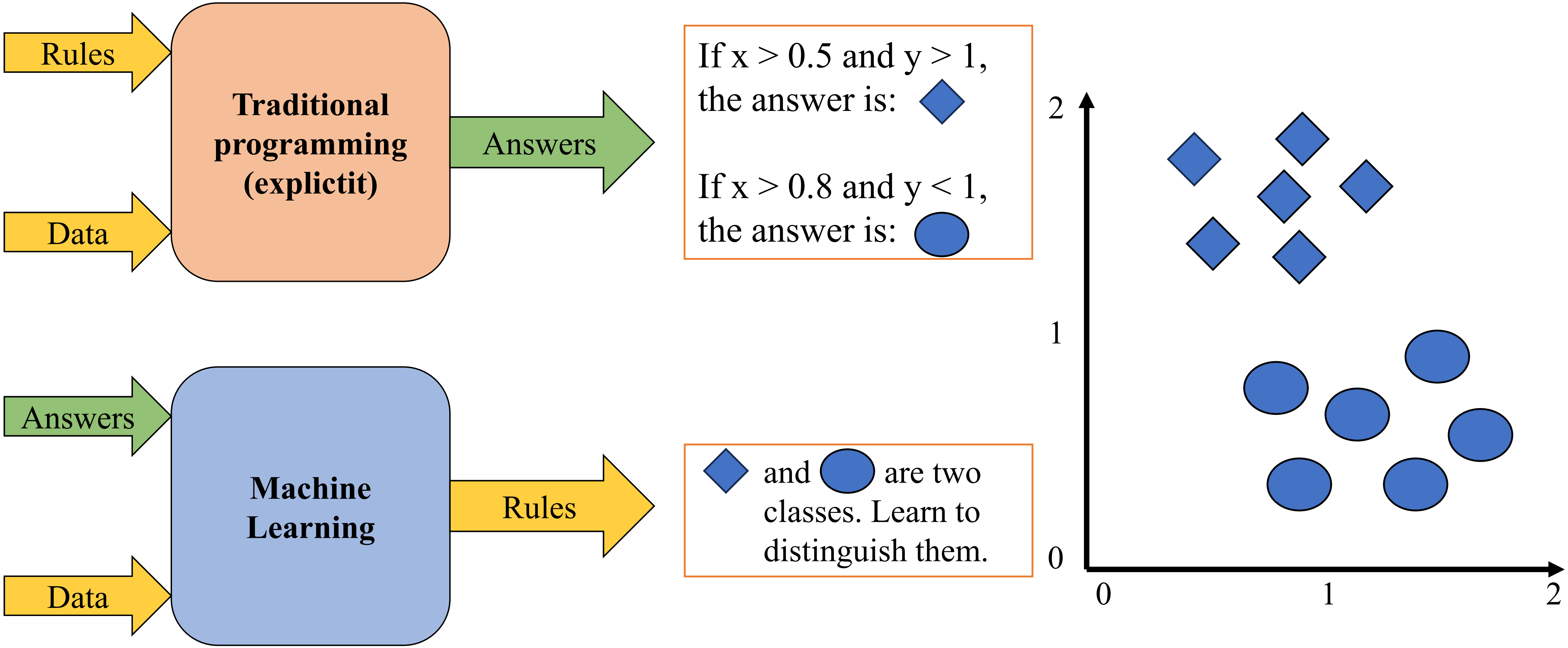
What are Artificial Neural Networks?

ML = Technique that allows a machine to learn without being explicitly programmed

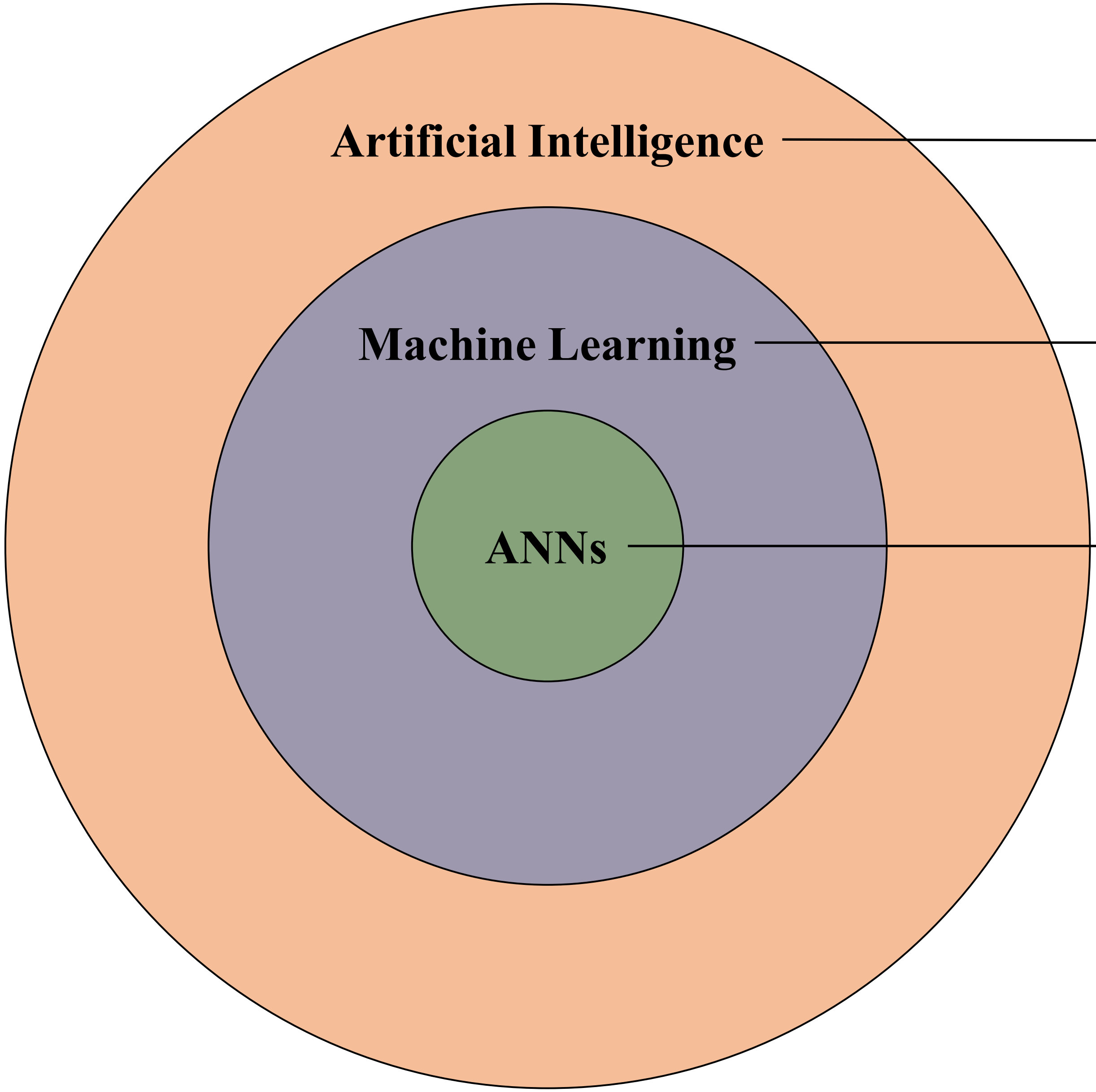


What are Artificial Neural Networks?

ML = Technique that allows a machine to learn without being explicitly programmed



What are Artificial Neural Networks?

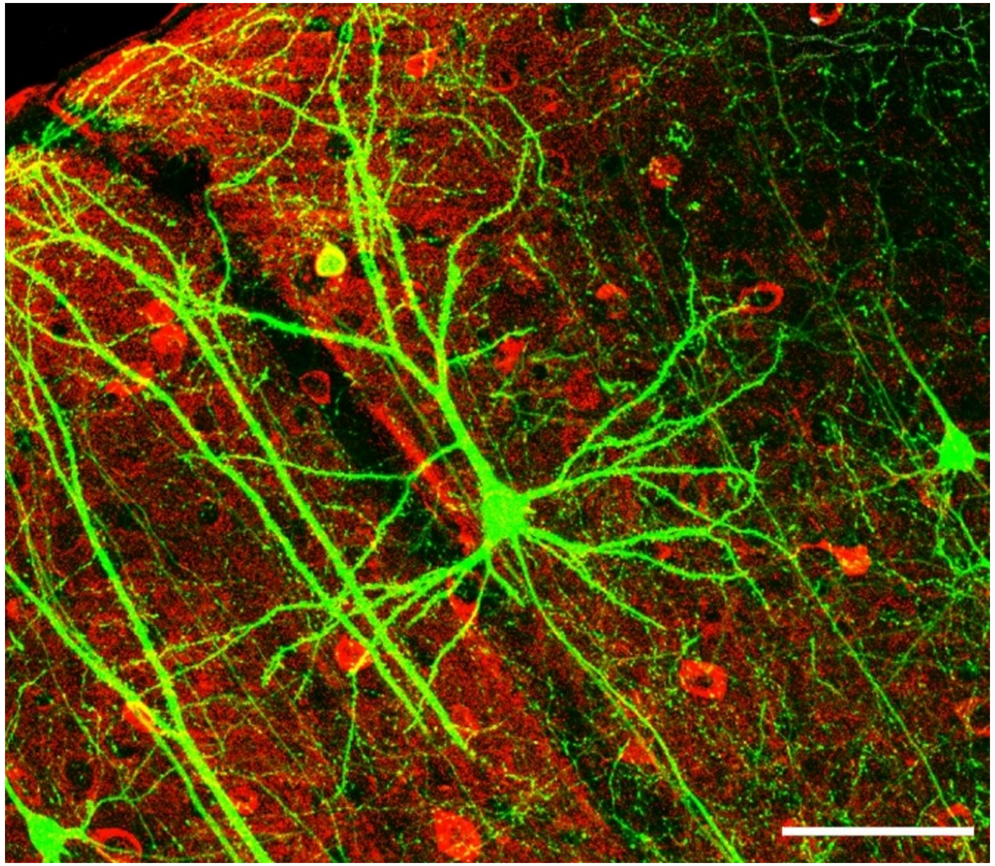


AI = Techniques that allow computers to mimic the behavior of human beings

ML = Technique that allows a machine to learn without being explicitly programmed

ANN = ML technique based on the architecture of biological neural networks

What are Artificial Neural Networks?



Wei-Chung Allen Lee, Hayden Huang, Guoping Feng, Joshua R. Sanes, Emery N. Brown, Peter T. So, Elly Nedivi, PLoSBiol4.e126.Fig6fNeuron, CC BY 2.5

1. **Neurons (units):** Basic processing unit.
2. **Connectivity:** Neurons are connected to each other.
3. **Activation:** Neurons „fire“ after exceeding threshold.
4. **Layers:** Neurons are organized in layers.
5. **Feedforward information flow:** From input to output.
6. **Feedback information flow:** From output to input.
7. **Learning and Adaptation:** Adapting connections to stimuli.
8. **Parallel processing:** Processing information simultaneously.

What are Artificial Neural Networks?

1. Data

Zxb, Storage size comparison, CC BY-SA 2.0 AT

2. Hardware

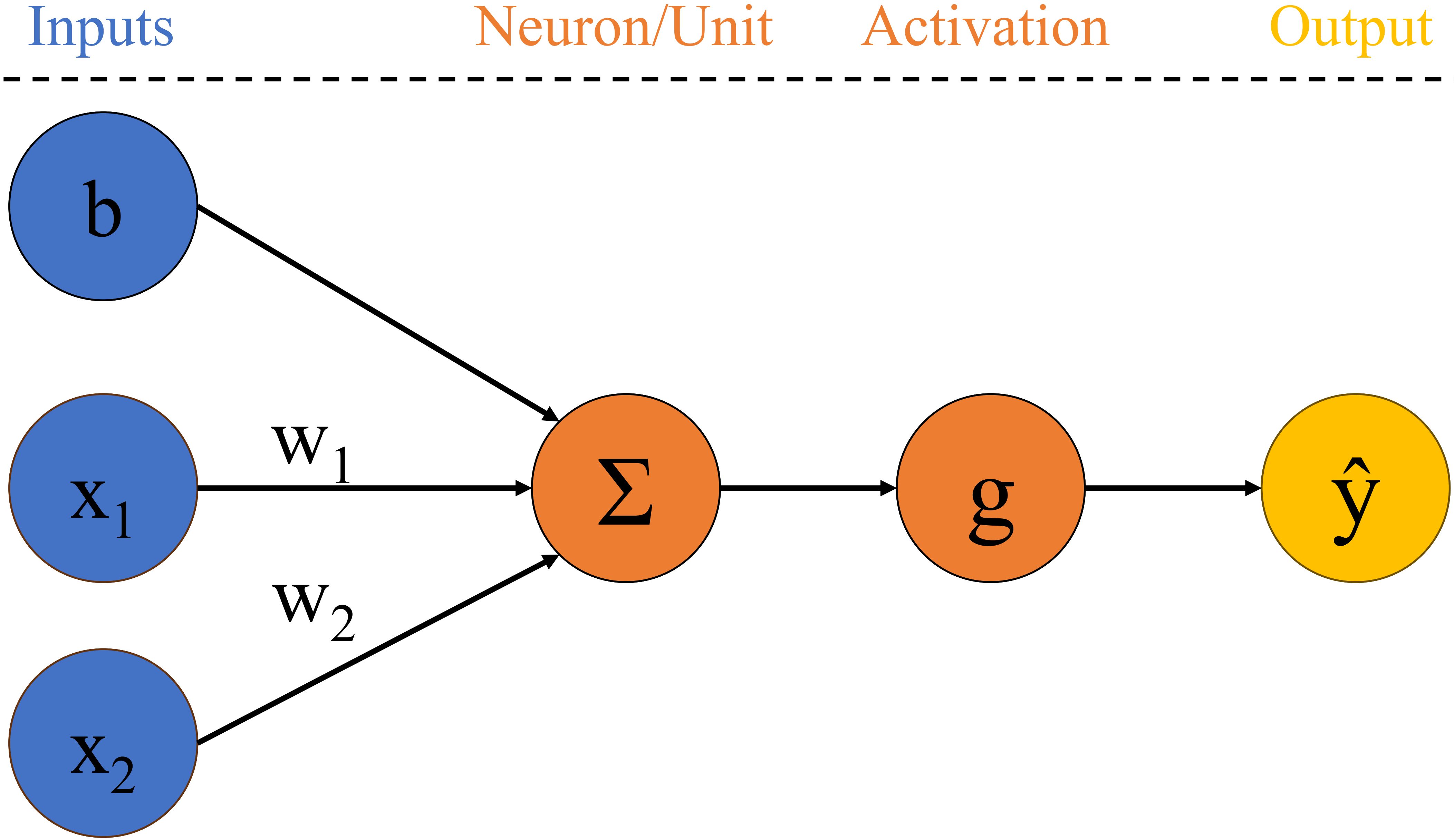
A7N8X, Xbox GPU, CC BY-SA 4.0

3. Software

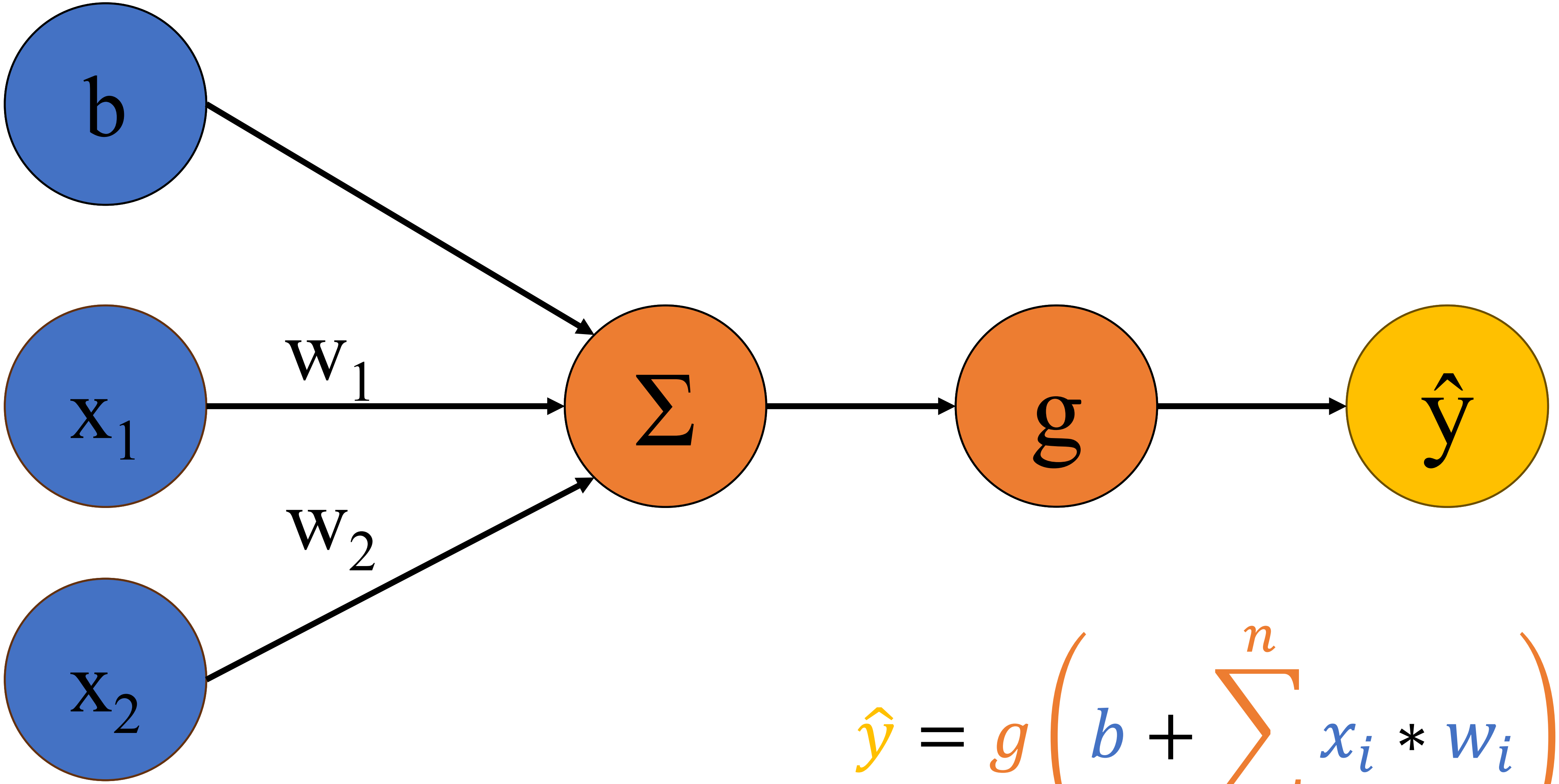
vscode-icons, Pytorch-svgrepo-com, CC BY-SA 4.0

vscode-icons, Tensorflow-svgrepo-com, CC BY-SA 4.0

What is an Artificial Neuron?

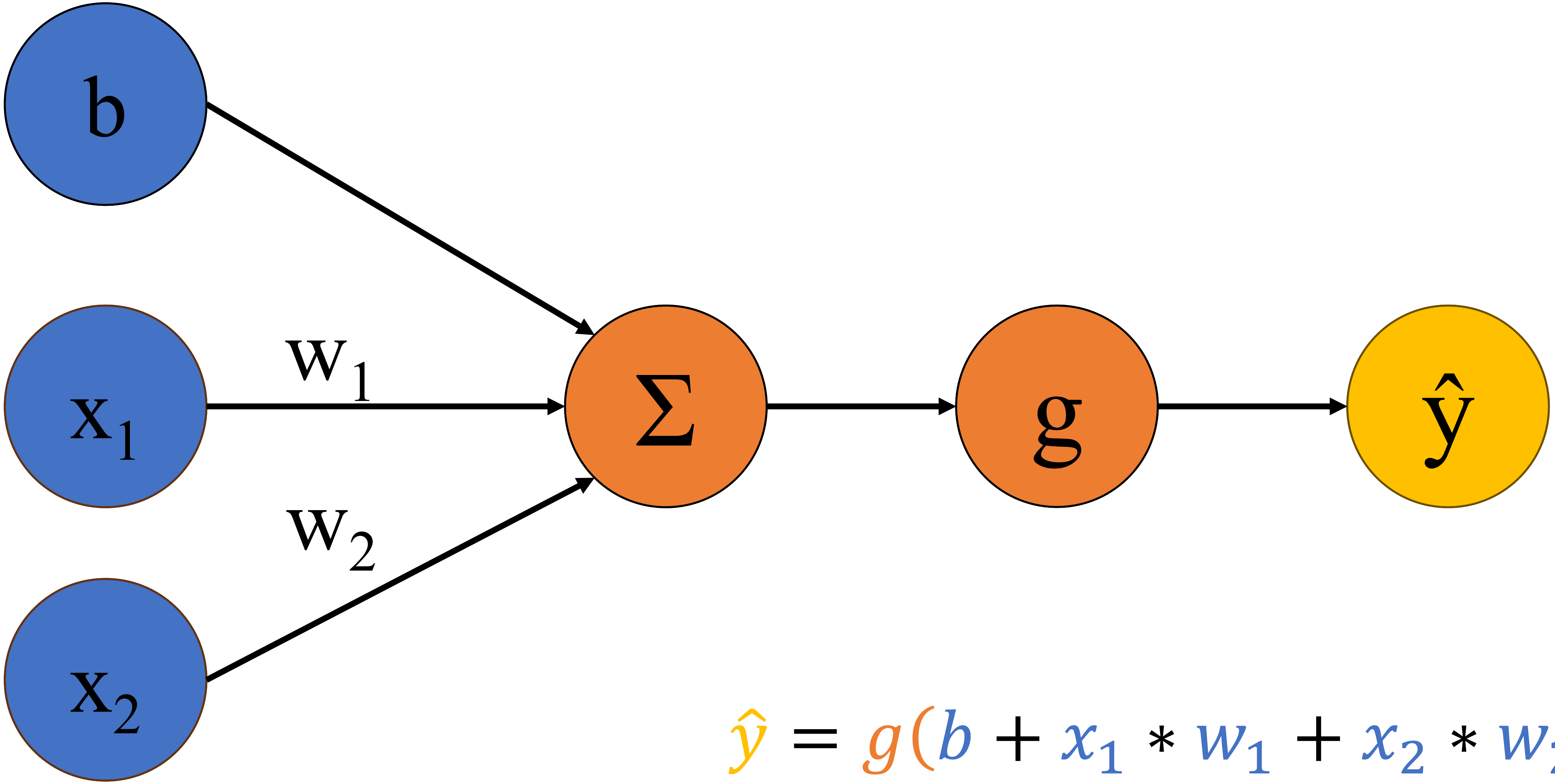


What is an Artificial Neuron?



$$\hat{y} = g\left(b + \sum_{i=1}^{n} x_i * w_i\right)$$

What is an Artificial Neuron?



$$\hat{y} = g(b + x_1 * w_1 + x_2 * w_2)$$

What is an Artificial Neuron?

Example: Oktoberfest

Heribert Pohl --- Thanks for half a million clicks! from Germering bei München, Bayern, O'zapft is! Münchens 5 Jahreszeit hat begonnen - O'zapft is! Munich 5 season, the Oktoberfest has begun (9855483374), CC BY-SA 2.0

Prediction: Are you going to the Oktoberfest this Saturday?

Criteria (weights):

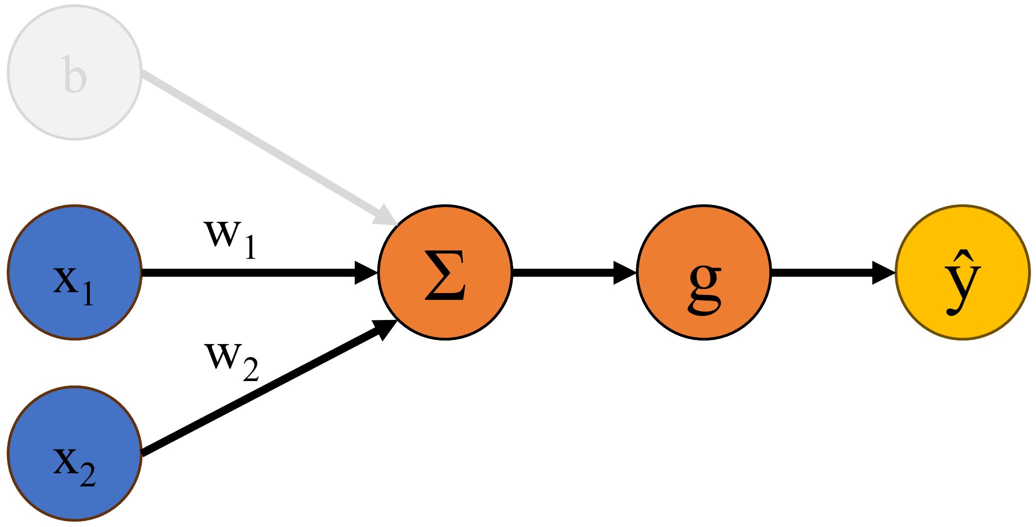
1. Do you like beer?
    - Yes (1) – No (0)
2. How important is the weather to you?
    - Very (1) – Not at all (0)

What is an Artificial Neuron?

Prediction: Are you going to the Oktoberfest this Saturday?

Criteria (weights):

1. Do you like beer?
   - Yes (1) – No (0)
2. How important is the weather to you?
   - Very (1) – Not at all (0)



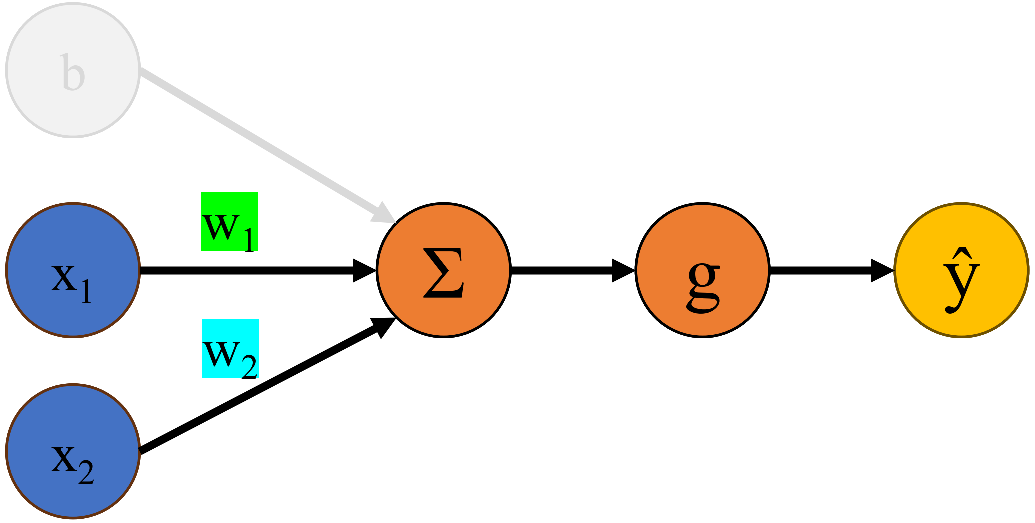
$$\hat{y} = g(x_1 * w_1 + x_2 * w_2)$$

What is an Artificial Neuron?

Prediction: Are you going to the Oktoberfest this Saturday?

Criteria:

1. Do you like beer?
   - Yes (1) – No (0)
2. How important is the weather to you?
   - Very (1) – Not at all (0)



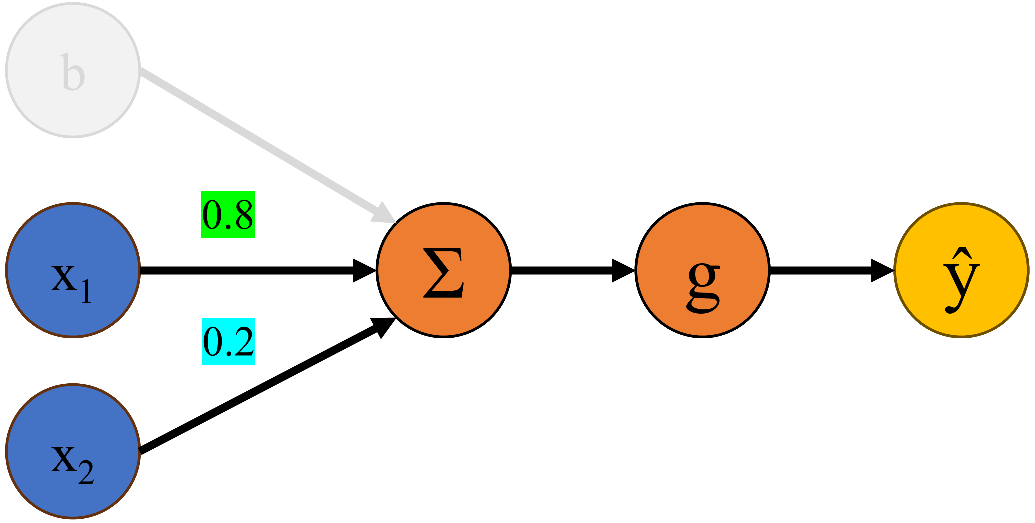
$$\hat{y} = g(x_1 * w_1 + x_2 * w_2)$$

What is an Artificial Neuron?

Prediction: Are you going to the Oktoberfest this Saturday?

Person 1:

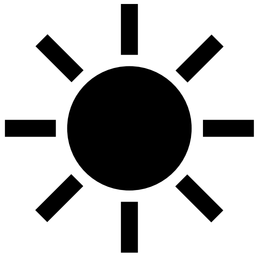
1. Do you like beer?
   - „Pretty much" (0.8)
2. How important is the weather to you?
   - "There is no bad weather, only the wrong clothes" (0.2)



$$\hat{y} = g(x_1 * 0.8 + x_2 * 0.2)$$

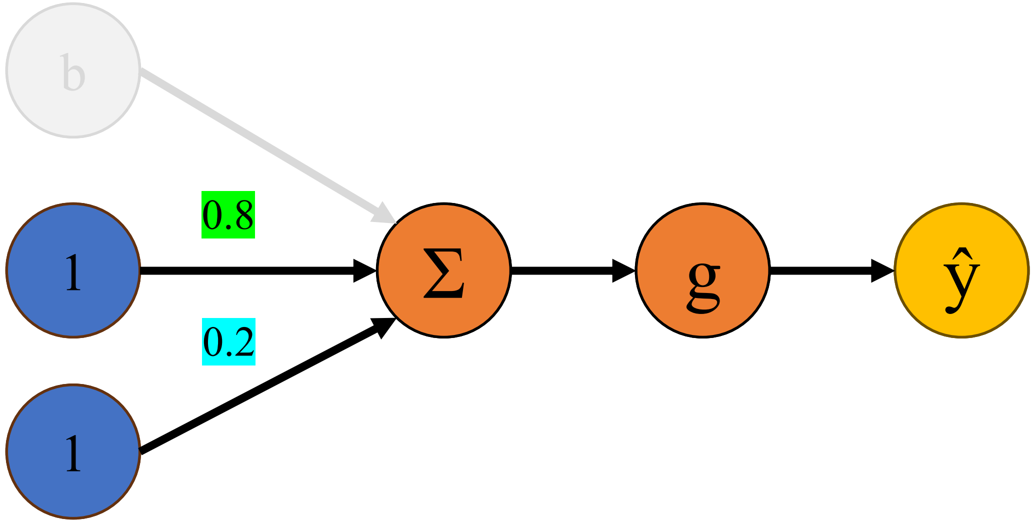
What is an Artificial Neuron?

Prediction: Are you going to the Oktoberfest this Saturday?



Person 1:

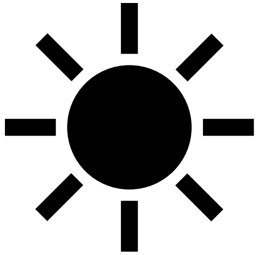
1. Do you like beer?
   - „Pretty much“ (0.8)
2. How important is the weather to you?
   - “There is no bad weather, only the wrong clothes” (0.2)



$$\hat{y} = g(1 * 0.8 + 1 * 0.2)$$
$$\hat{y} = g(1)$$

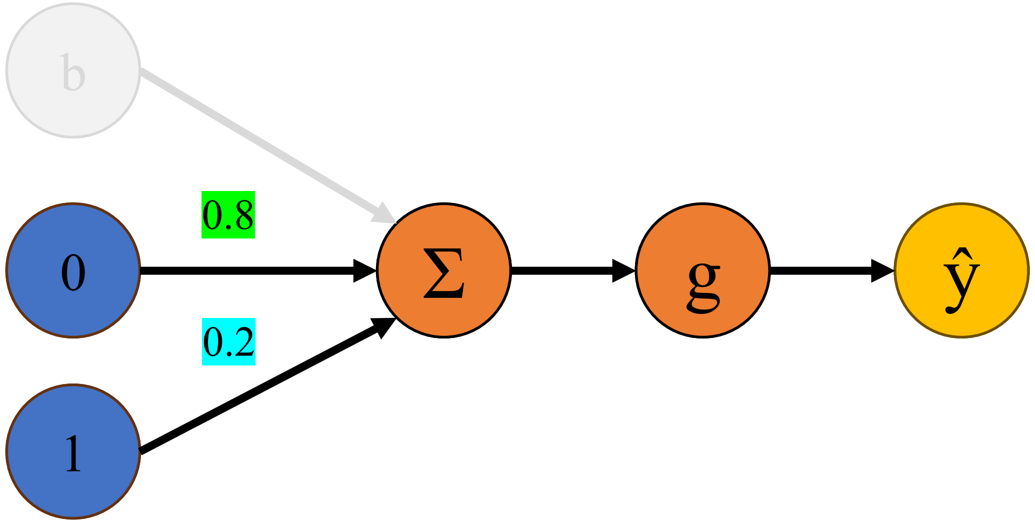
What is an Artificial Neuron?

Prediction: Are you going to the Oktoberfest this Saturday?



Person 1:

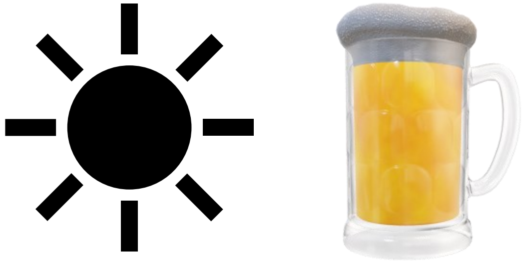
1. Do you like beer?
   - „Pretty much“ (0.8)
2. How important is the weather to you?
   - “There is no bad weather, only the wrong clothes” (0.2)



$$\hat{y} = g(0 * 0.8 + 1 * 0.2)$$
$$\hat{y} = g(0.2)$$

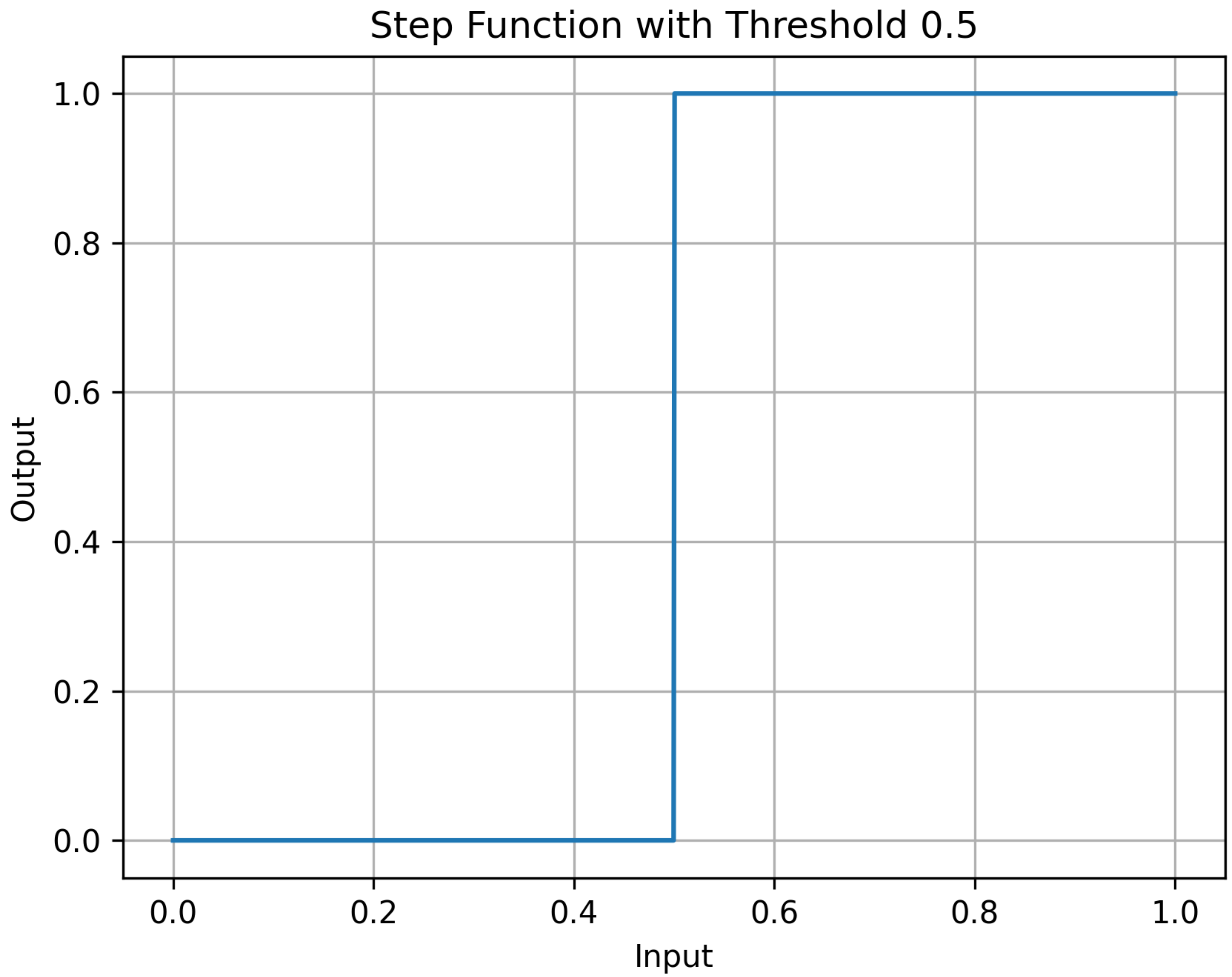
What is an Artificial Neuron?

Prediction: Are you going to the Oktoberfest this Saturday?

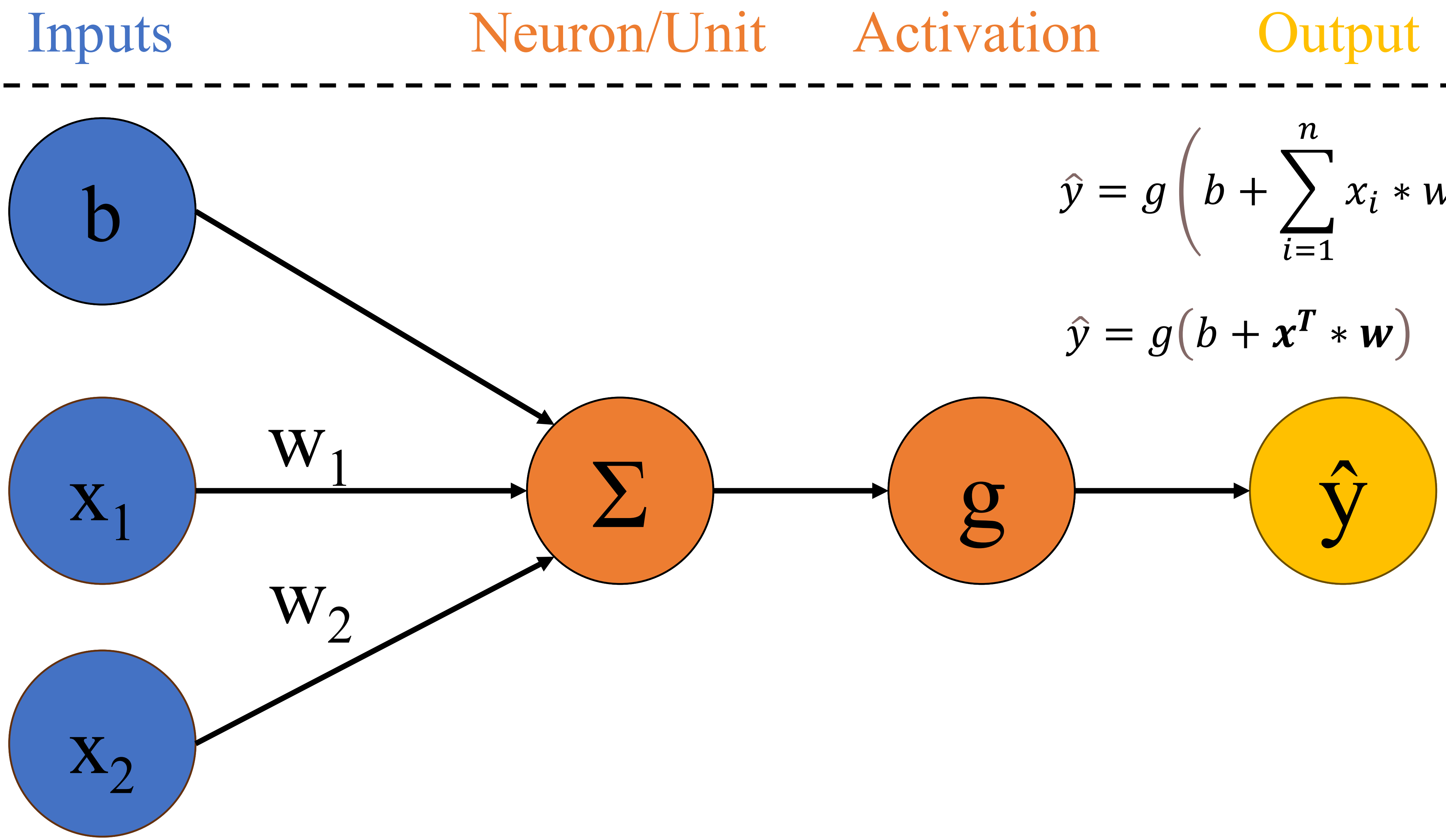


$$\hat{y} = g(1 * 0.8 + 1 * 0.2)$$
$$\hat{y} = g(1)$$

$$\hat{y} = g(0 * 0.8 + 1 * 0.2)$$
$$\hat{y} = g(0.2)$$



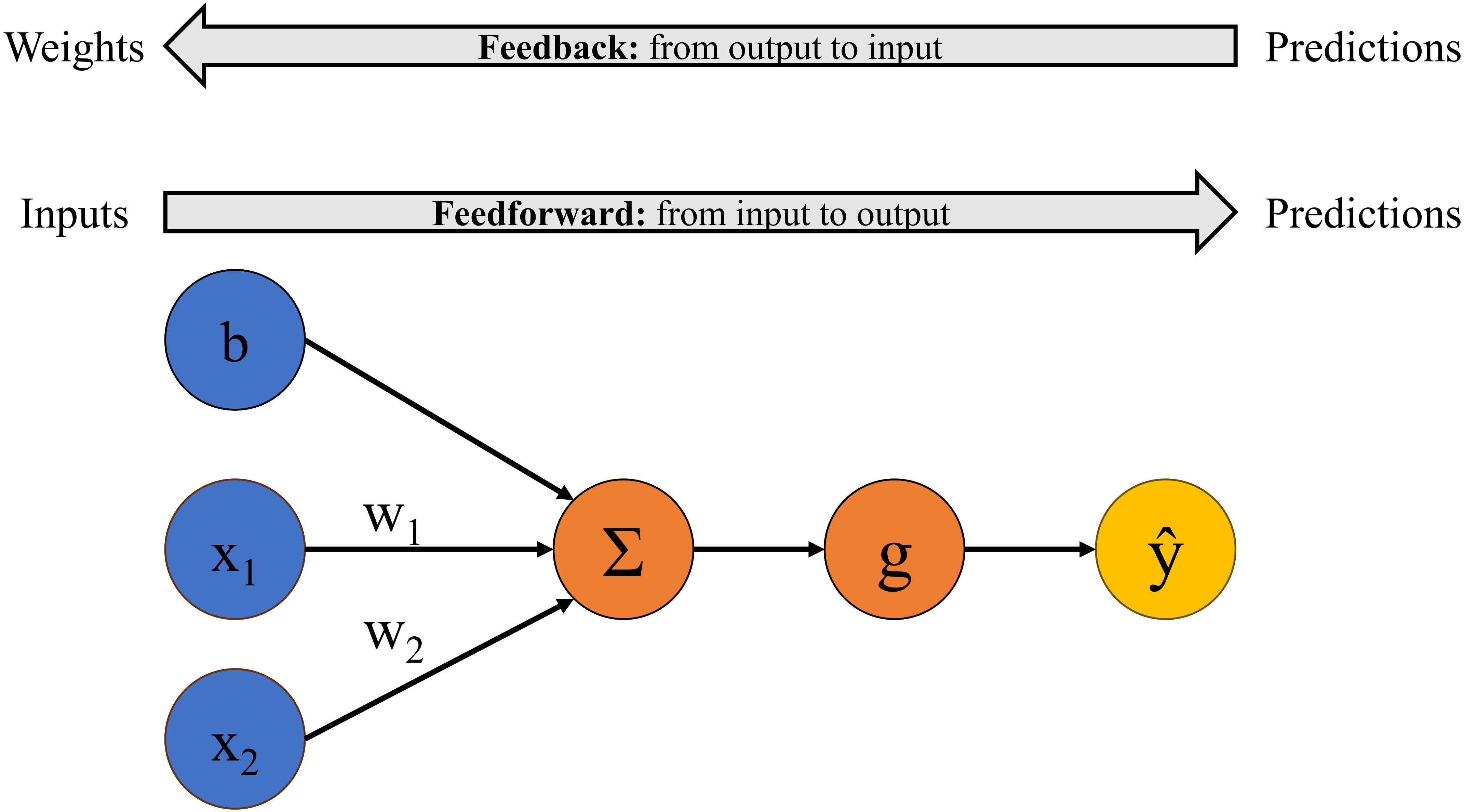
What is an Artificial Neuron?



$$\hat{y} = g\left(b + \sum_{i=1}^{n} x_i * w_i\right)$$

$$\hat{y} = g\left(b + \boldsymbol{x}^{\boldsymbol{T}} * \boldsymbol{w}\right)$$

How Do Artificial Neurons Learn?



How Do Artificial Neurons Learn?

Loss functions measure difference between true values (y) and predicted values (ŷ):

- Mean Absolute Error (MAE)
- Mean Squared Error (MSE)
- Binary Crossentropy
- Categorical Crossentropy
- …

$$\sum_{i=1}^{n} \frac{|\,\hat{y}_i - y_i\,|}{n}$$

$$\sum_{i=1}^{n} \frac{y_i * \log\big(p(y_i)\big) + (1 - y_i) * (\log(1 - p(y_i))}{n}$$

$\boldsymbol{p(y_i)}$ = Probability the model assigns the value to be ŷ

How Do Artificial Neurons Learn?

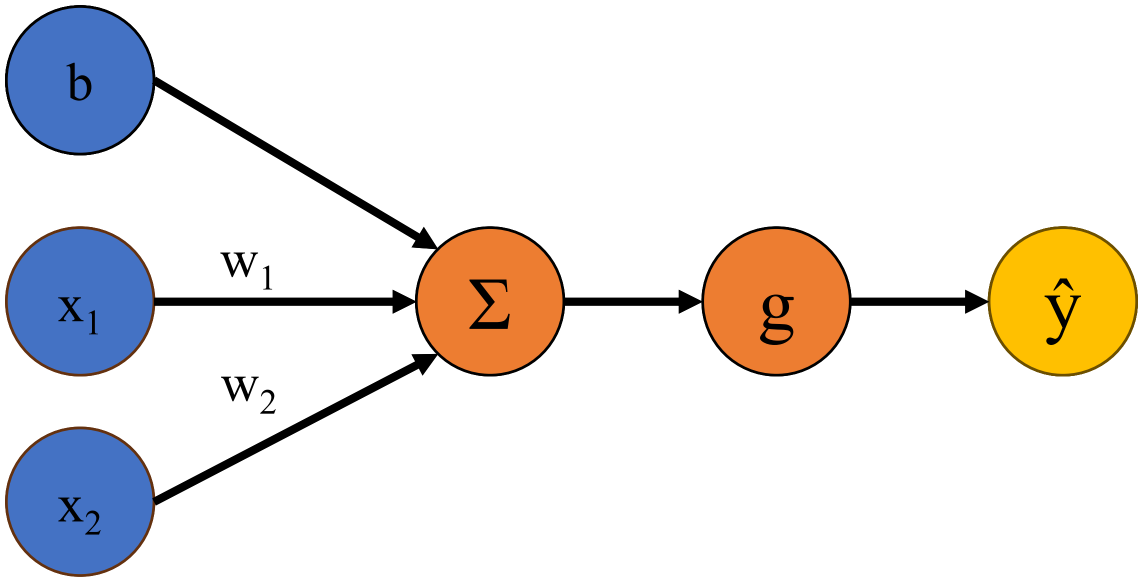
Loss functions measure difference between true values (y) and predicted values (ŷ):

- Mean Absolute Error (MAE)
- Mean Squared Error (MSE)
- Binary Crossentropy
- Categorical Crossentropy
- …

Training an artificial neuron (or network; learning) refers to the **minimization of the loss function**

The error is a function of all neurons, which in turn are a function of all weights. The error is **backpropagated** through the network and the weights are adjusted to minimize the loss function.

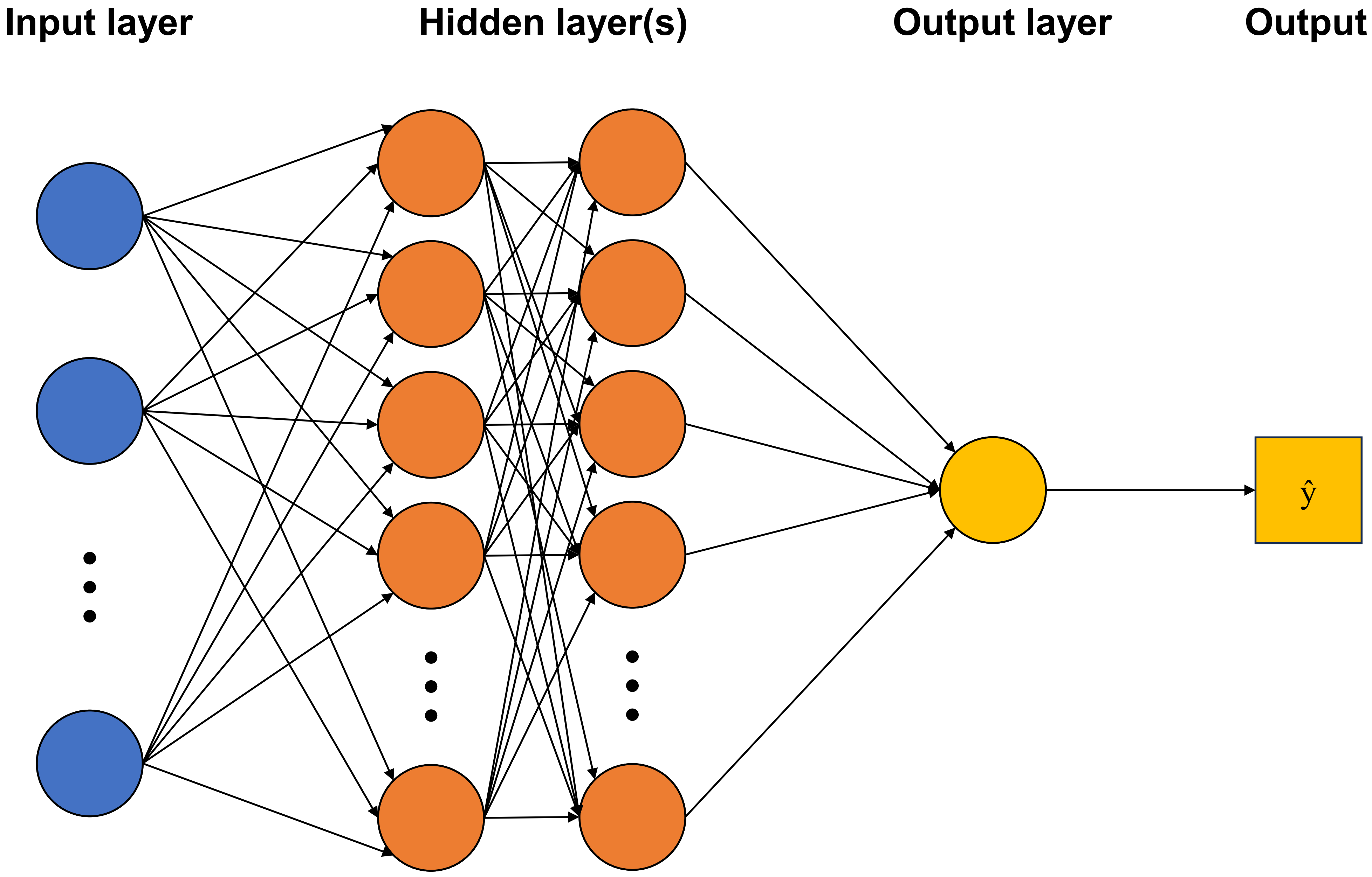
How Do Artificial Neurons Learn?



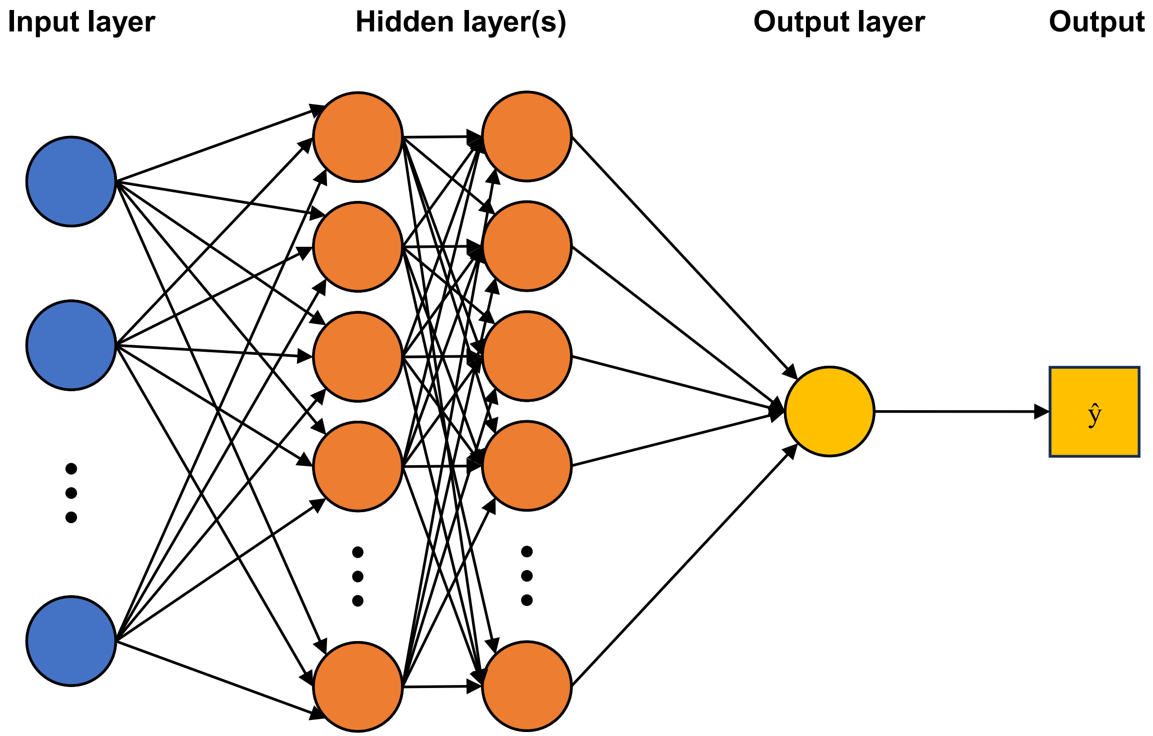
Training an artificial neuron (or network, learning) refers to the **minimization of the loss function**

The error is a function of all neurons, which in turn are a function of all weights. The error is **backpropagated** through the network and the weights are adjusted to minimize the loss function.

What is an Artificial Neural Network?



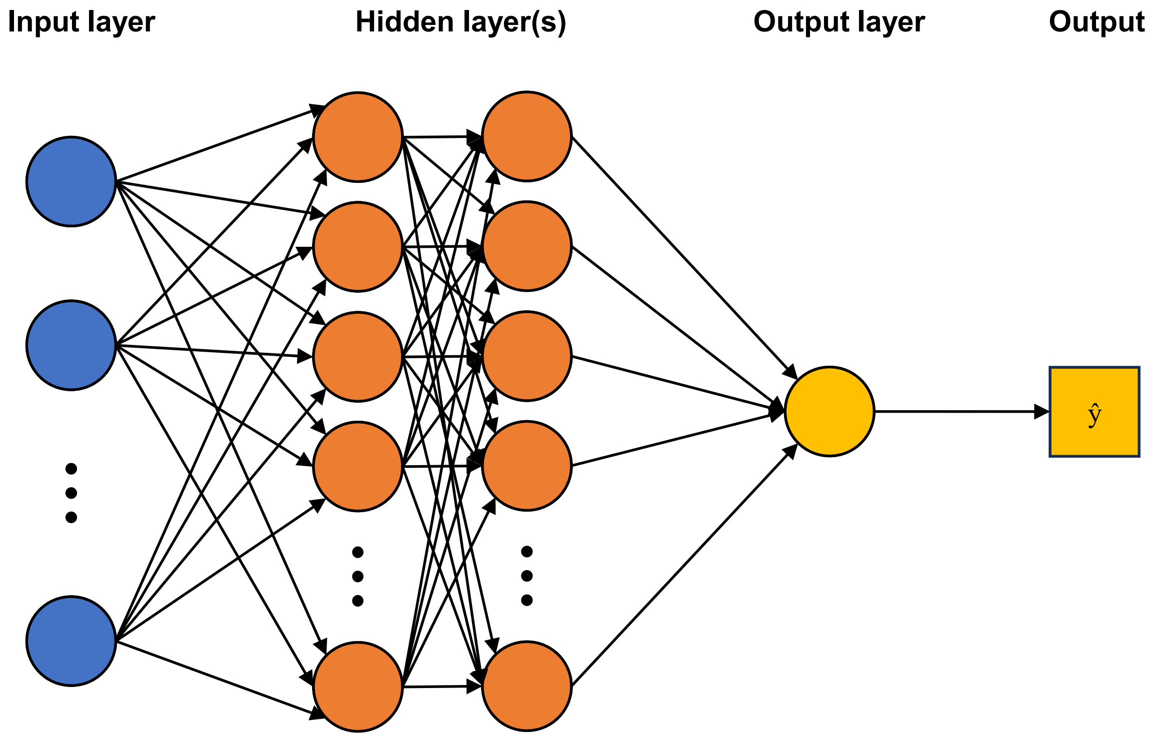
What is an Artificial Neural Network?



Universal approximation theorem: An ANN with enough neurons in the hidden layer can approximate any continuous function with arbitrary precision.

Deep Learning: Multiple hidden layers.

What is an Artificial Neural Network?

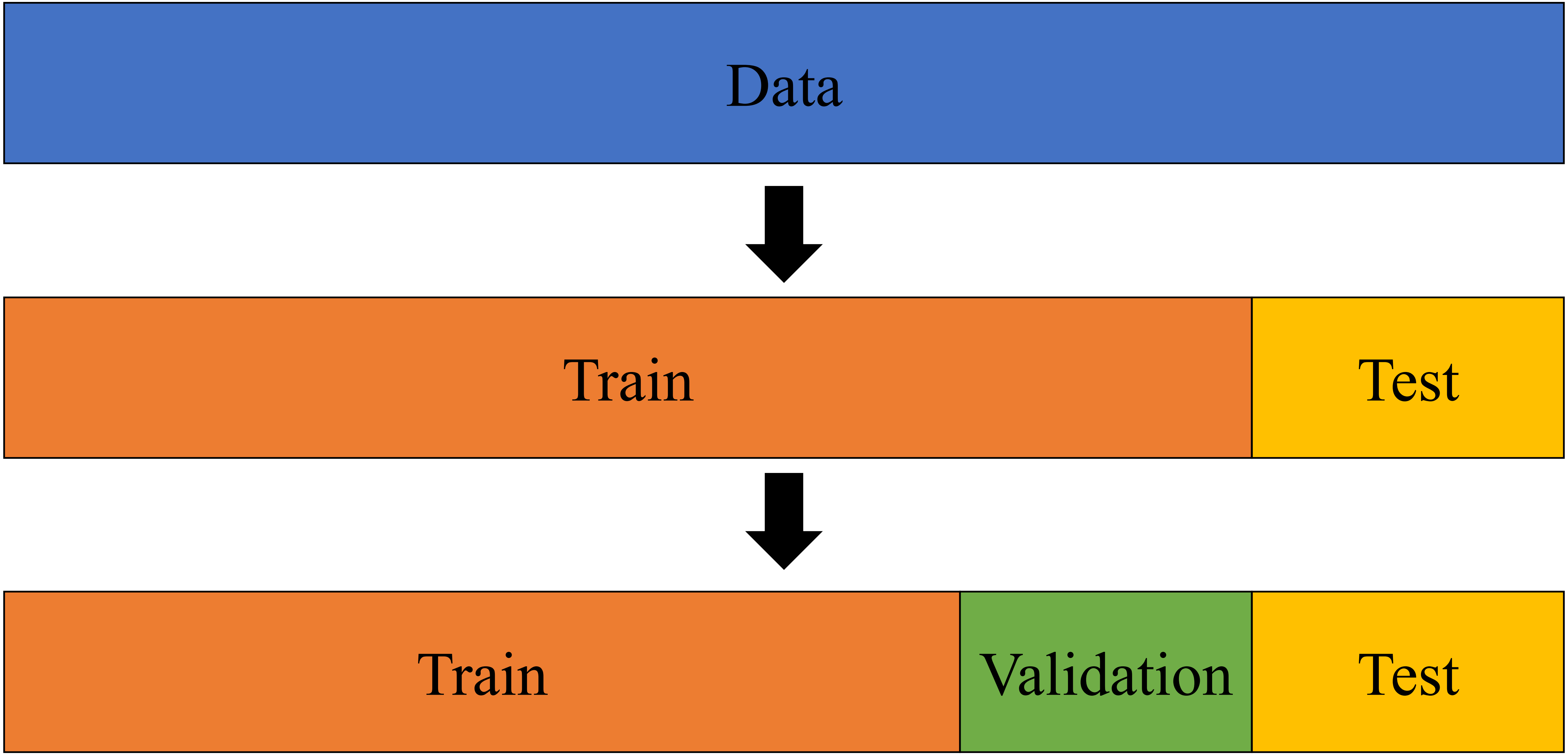


- Pattern Detector
- High-dimensional feature extractor
- Function approximator
- Computational model

Chapter 1 - Regression

- Regression model for Bradford assay
- Model for growth curve during diauxic growth
- Model for a circadian pattern of enzyme activity
- Human vs. Machine Learning
- The curse of small data sets
- Overfitting, Underfitting, and Holdout Validation

Holdout validation

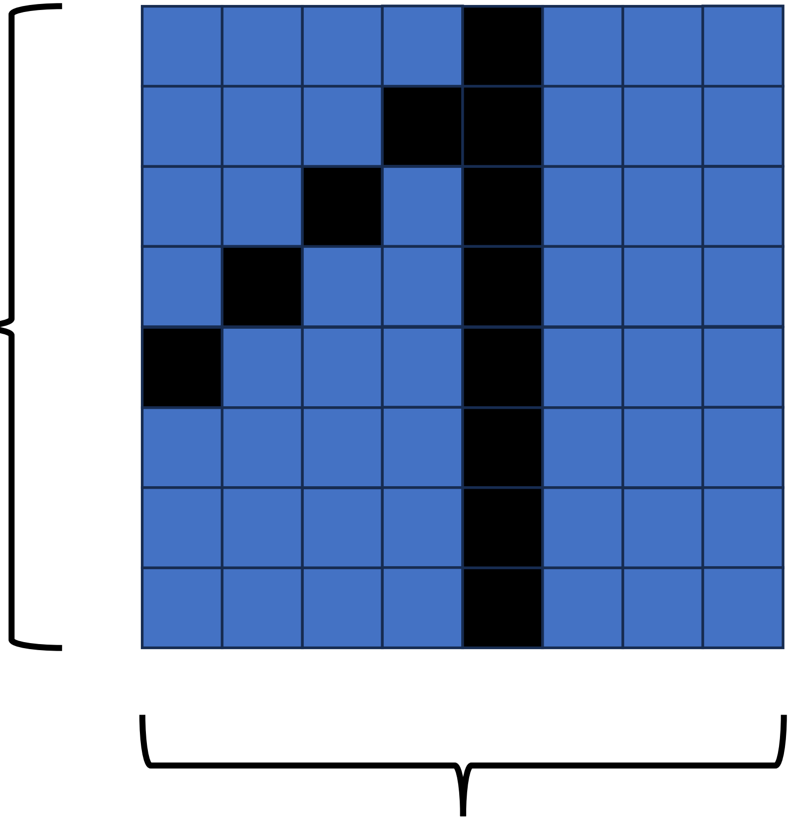


Chapter 2 - Classification

- Binary classification to distinguish microbial cells
- Multi-class classification to distinguish microbial cells
- Simple image classification using the MNIST dataset
- Precision and Recall, Confusion matrix and decision boundaries
- Black box problem

Multi-class classification network topology for images

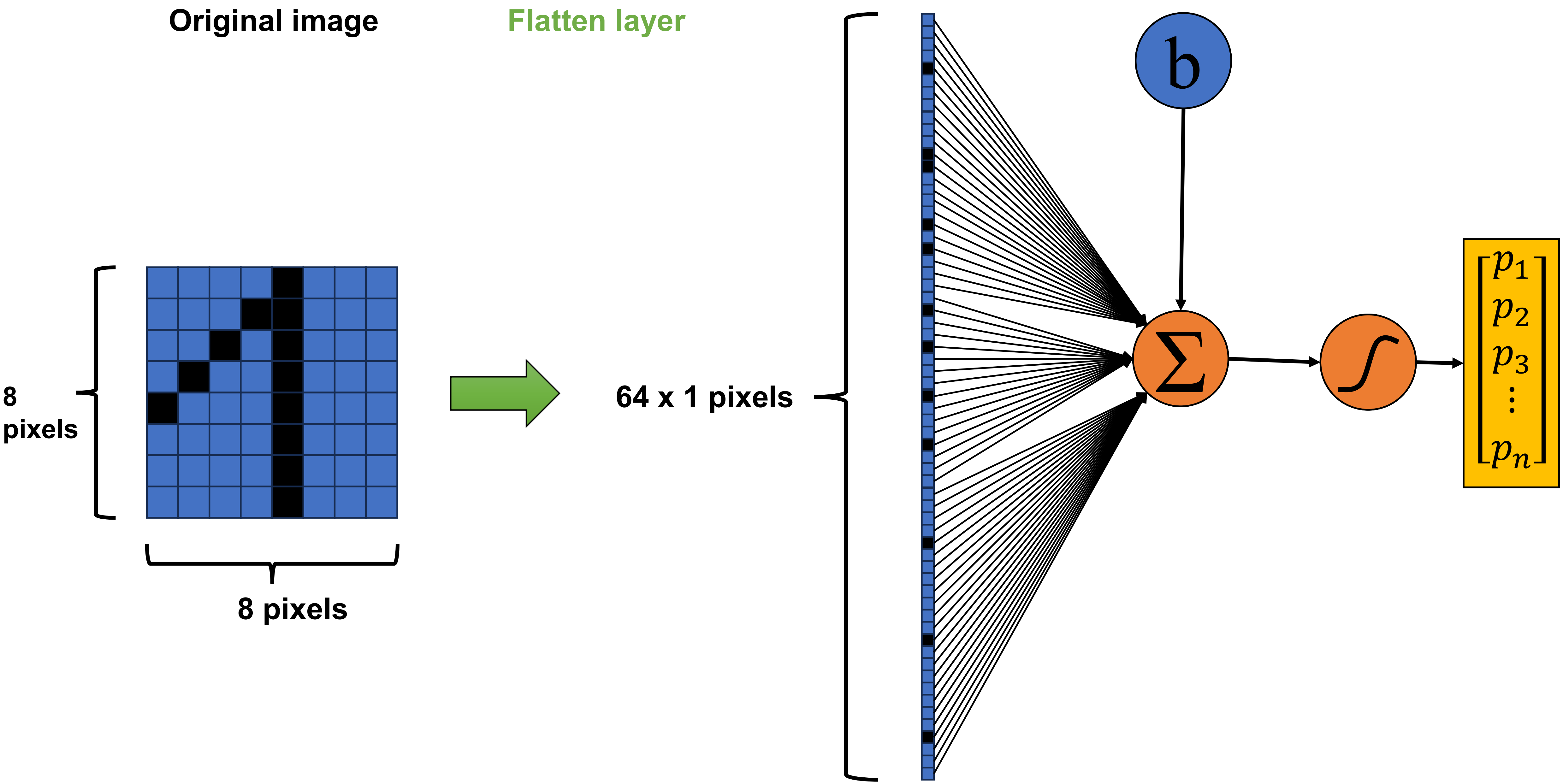
8 pixels



8 x 8 = 64 pixels total

8 pixels

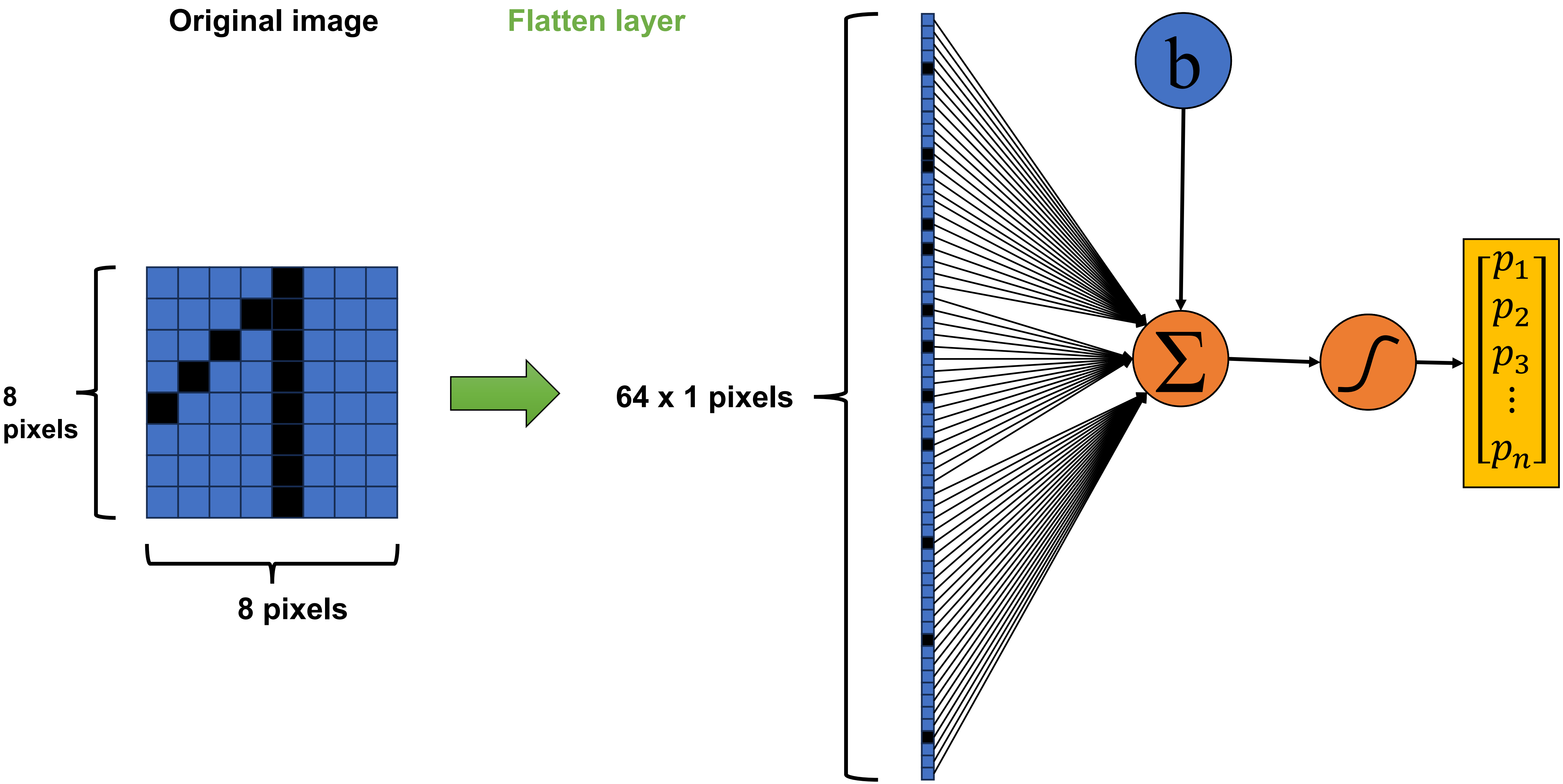
Multi-class classification network topology for images



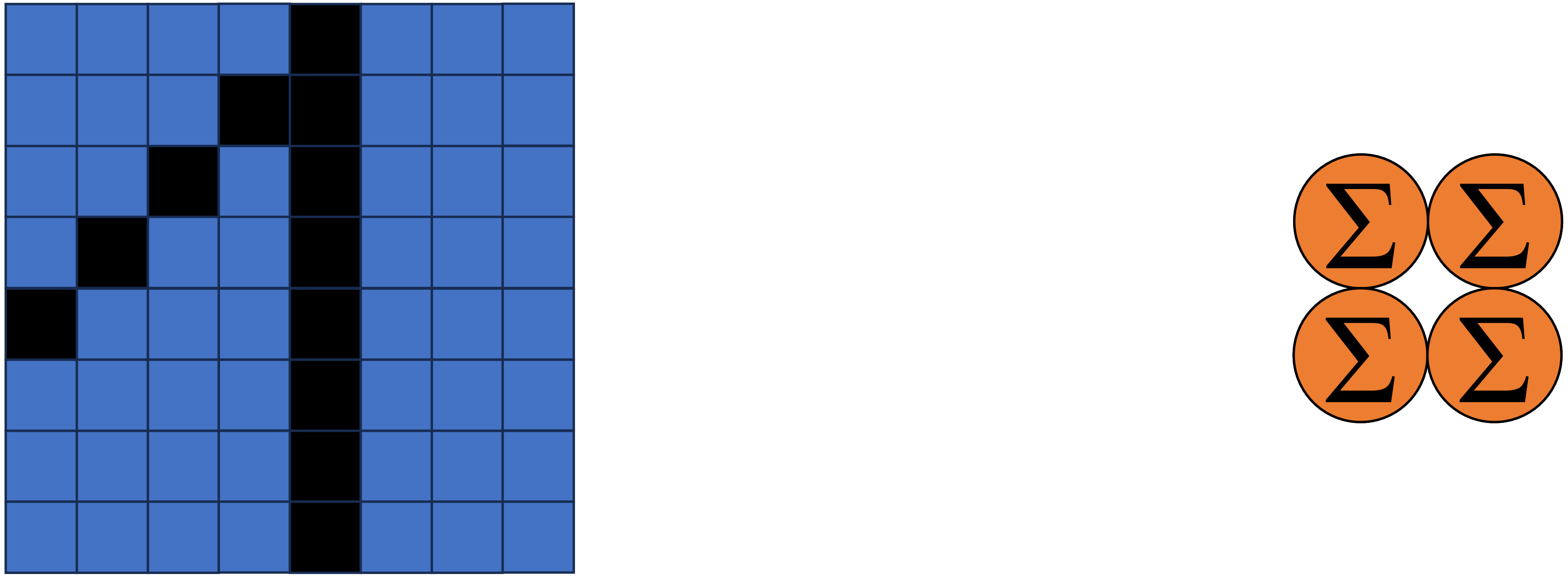
Chapter 3 – Convolutional Neural Networks

- CNN for healthy and infected cell classification
- Convolution layer and pooling layer
- Transfer learning

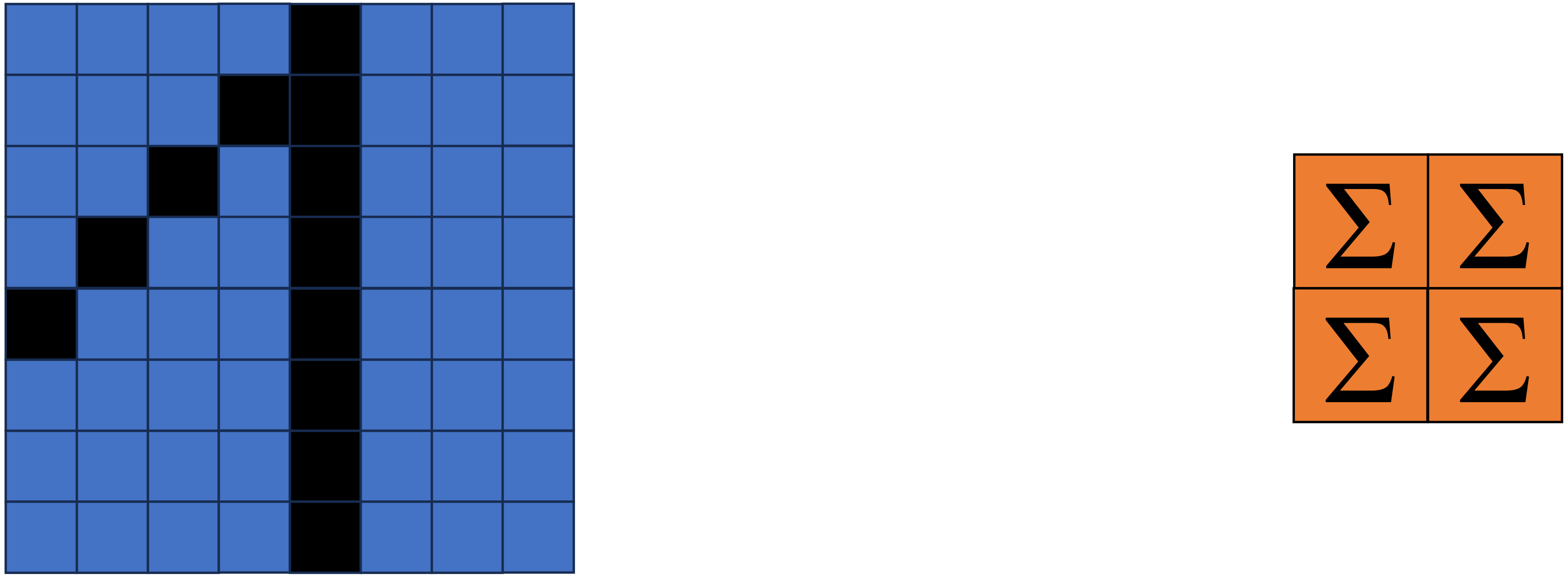
Multi-class classification network topology for images



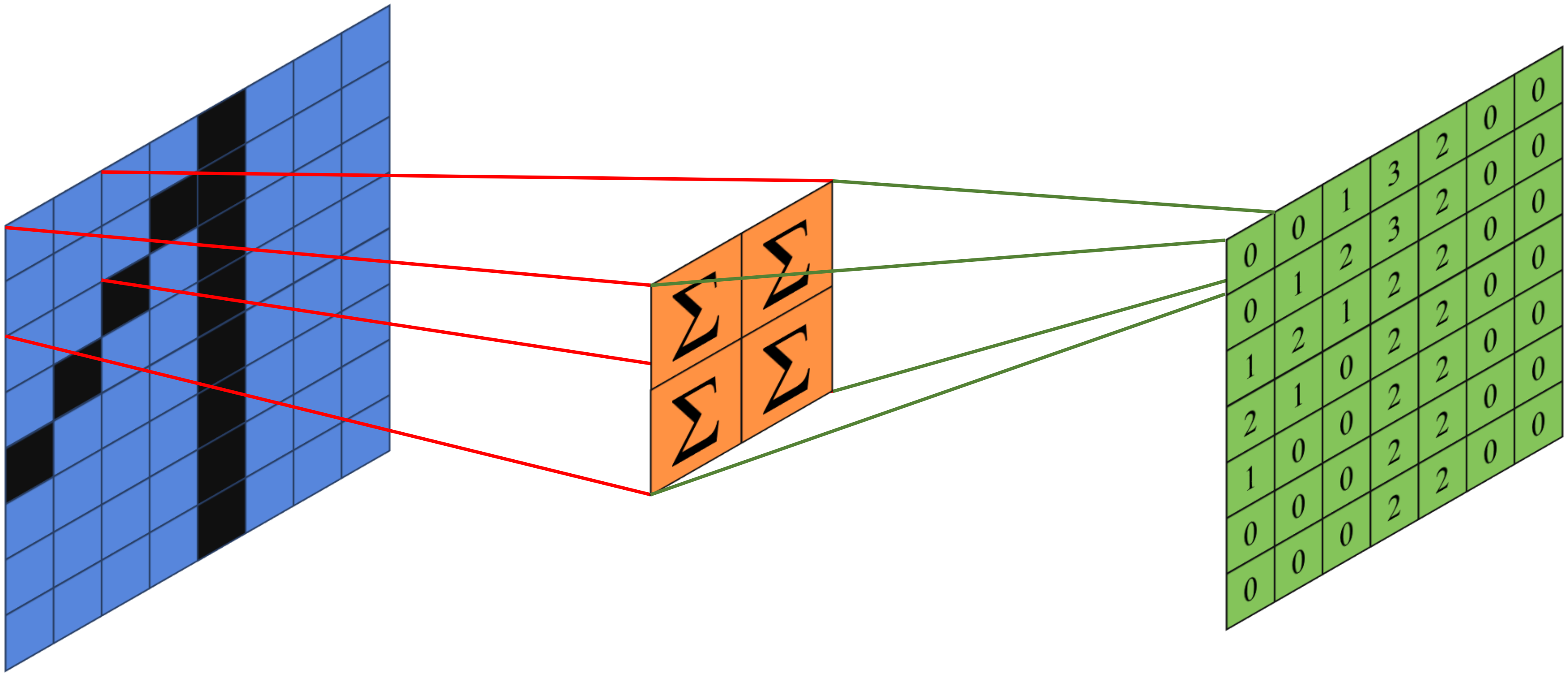
What is a Convolutional Layer?



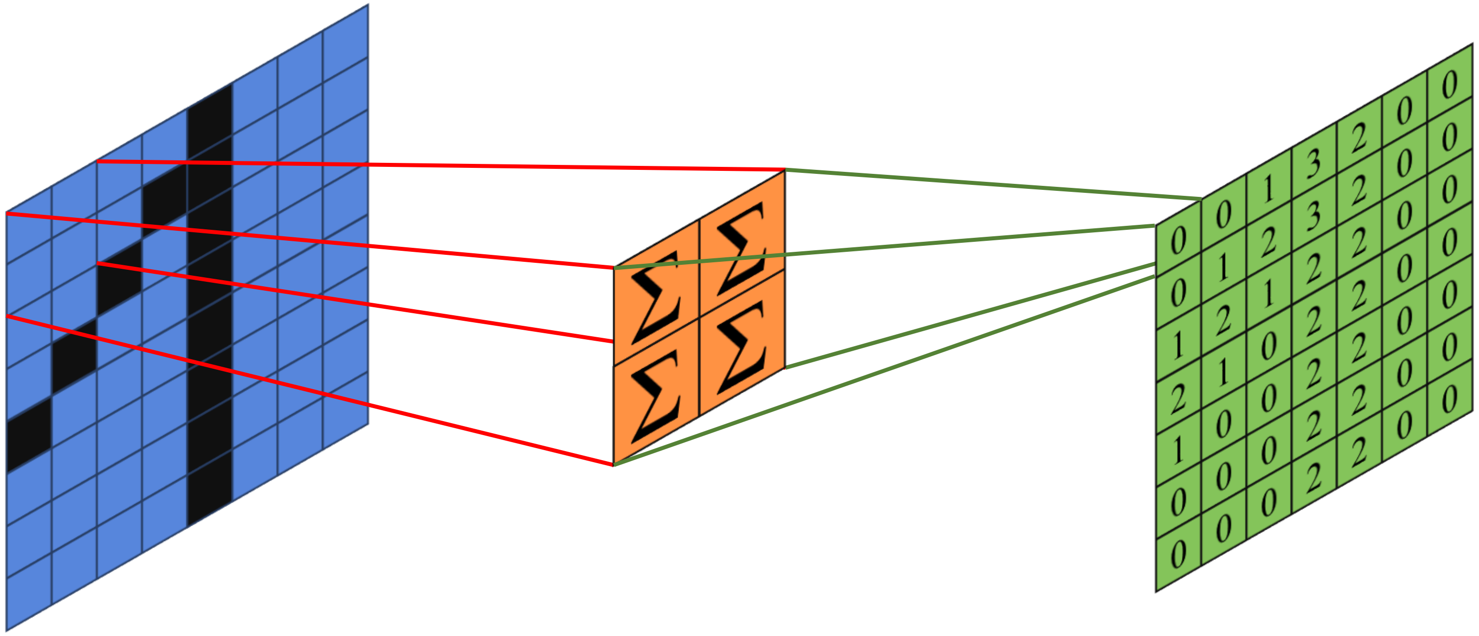
What is a Convolutional Layer?



What is a Convolutional Layer?



What is a Convolutional Layer?

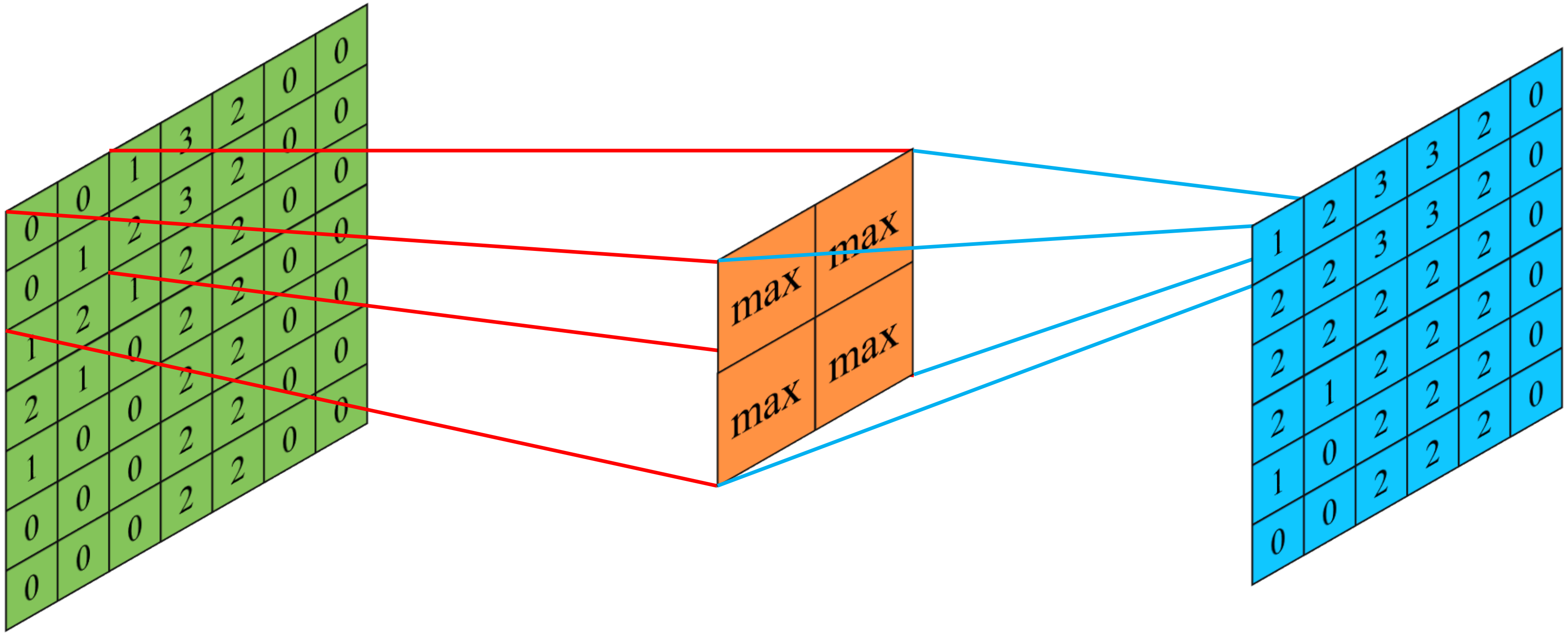


Convolutional layers preserve the intrinsic structure of the data. The output is called a **feature map**. As a result, they perform very well on **structured data**.

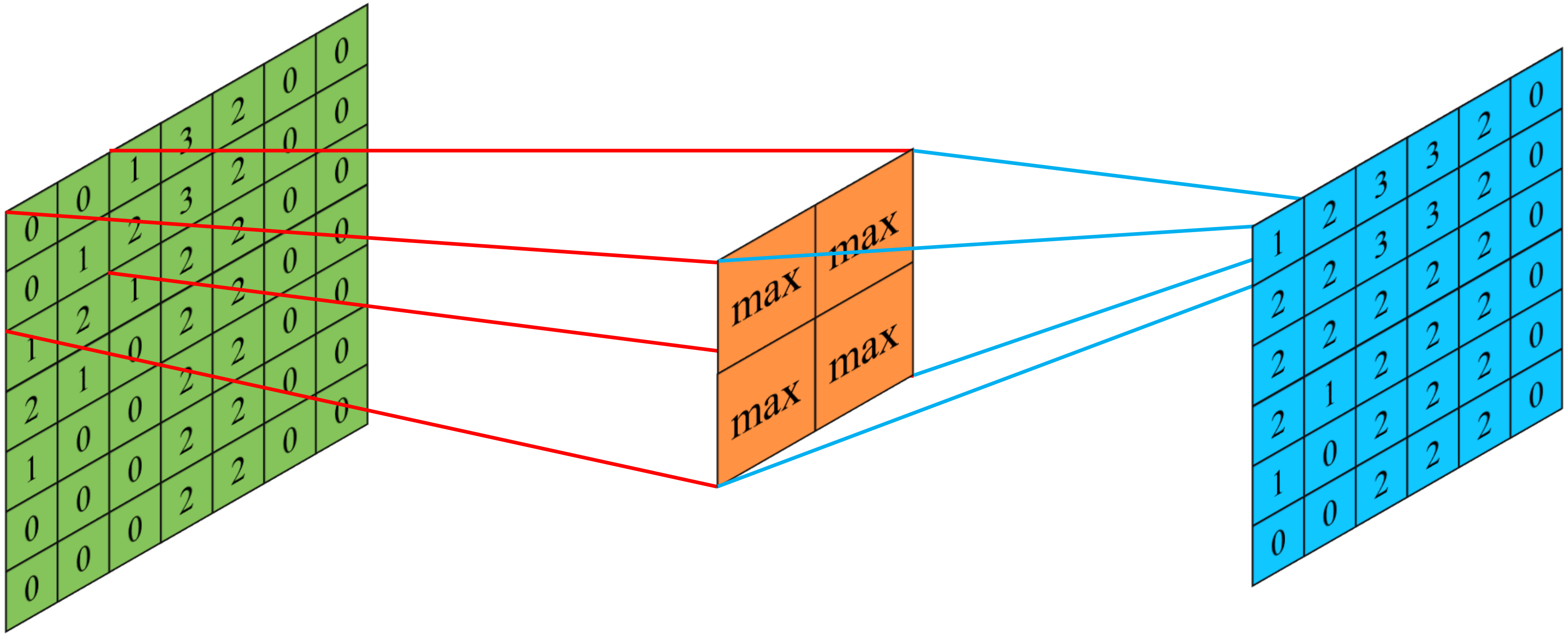
Examples include:

- Computer Vision
- Natural Language Processing
- Time series forecasting and classification
- Molecular structure prediction

What is a Pooling Layer?



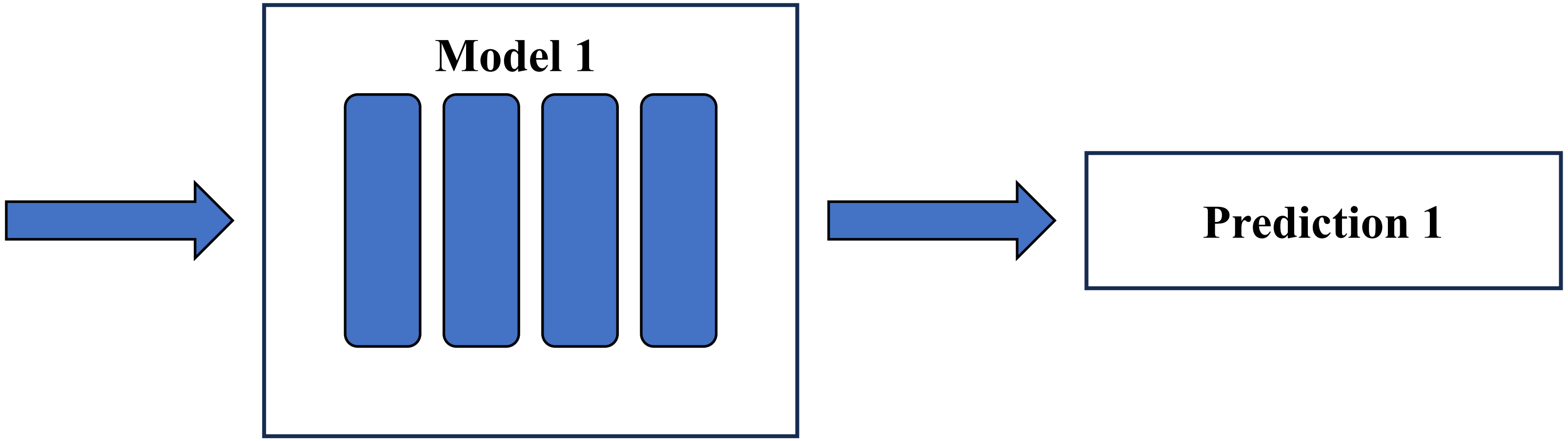
What is a Pooling Layer?



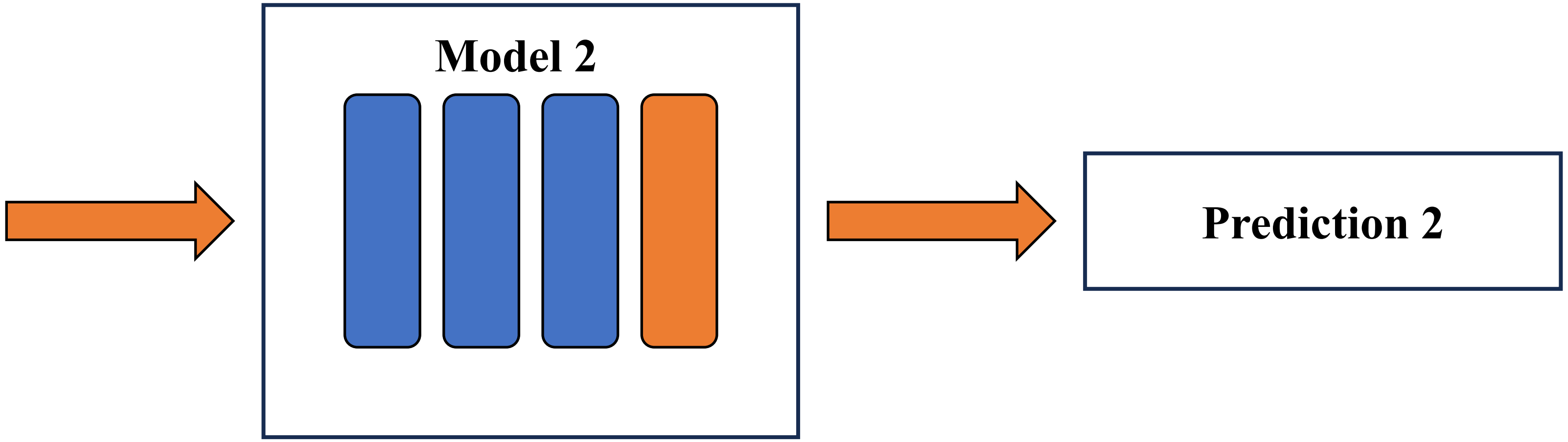
Pooling layers reduce the size of feature maps while preserving **meaningful features**.

What is Transfer Learning?

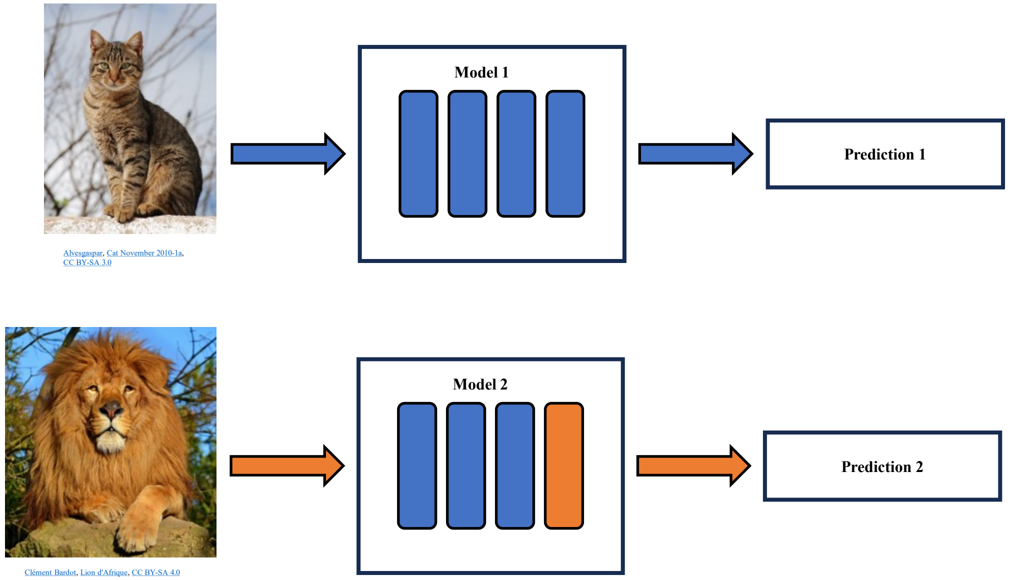
Alvesgaspar, Cat November 2010-1a, CC BY-SA 3.0



Clément Bardot, Lion d'Afrique, CC BY-SA 4.0



What is Transfer Learning?



Alvesgaspar, Cat November 2010-1a, CC BY-SA 3.0

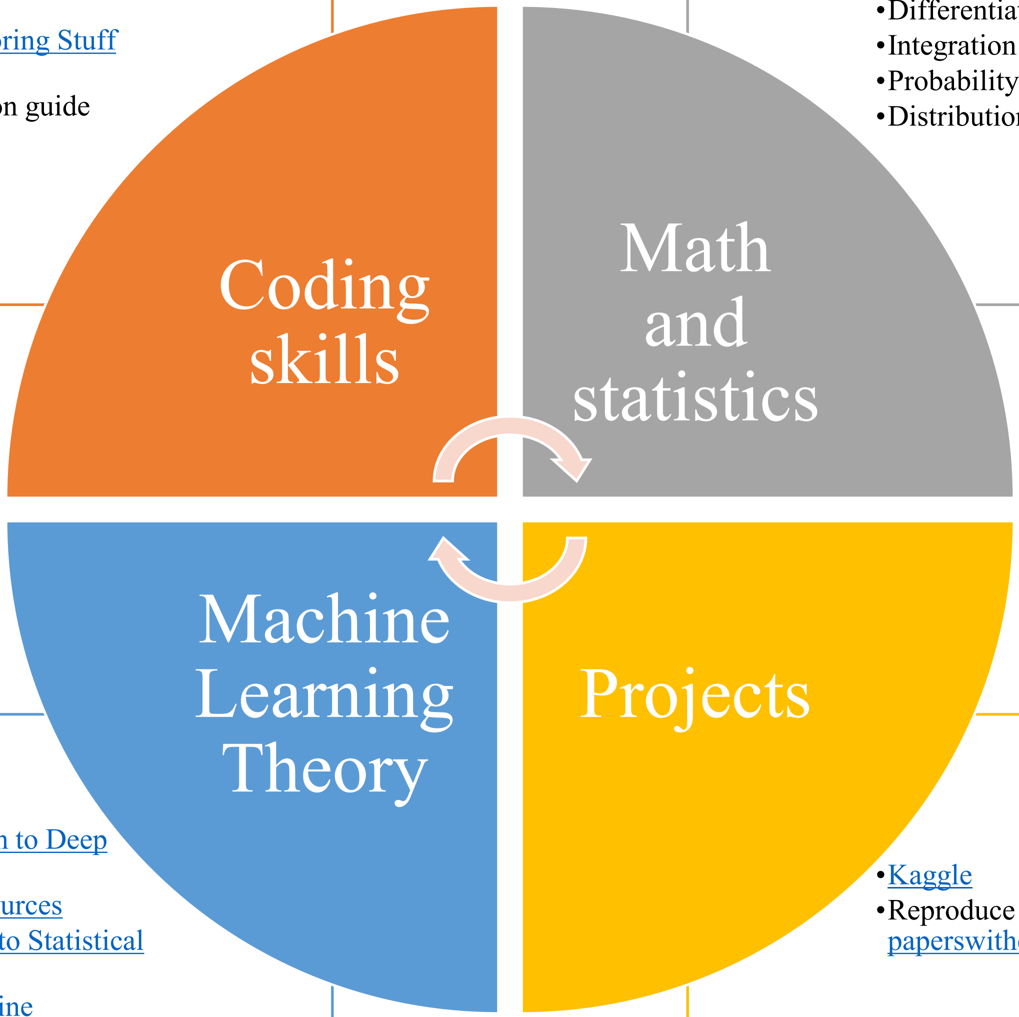
Clément Bardot, Lion d'Afrique, CC BY-SA 4.0

Transfer learning is a technique that uses a **pre-trained model** for a related task.

Benefits:

- **Faster training**
- **Improved performance** with small amount of data
- **Generalization**: Pre-trained models have typically learned general features

What next?



- Python books and courses at O'Reilly
- Automate the Boring Stuff with Python
- Interactive Python guide PyFlo

- Linear Algebra
- Differentiation
- Integration
- Probability
- Distributions

- MIT Introduction to Deep Learning
- TensorFlow resources
- An Introduction to Statistical Learning
- Hands-On Machine Learning

- Kaggle
- Reproduce paper using paperswithcode.com