

# COSC 325: Introduction to Machine Learning

Dr. Hector Santos-Villalobos



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# Lecture 20: Introduction to Artificial Neural Networks



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# Class Announcements

## Homework

Homework #6 is due Tomorrow Wednesday.

## Course Project:

Course Project Presentation Poster

- In-class 12/03
- Template available in Canvas
  - 24" Tall x 36" Wide
- Stitched copy paper is fine.

## Lectures:

**Next Lecture:** Tenure Teaching Evaluation

## Quizzes:

Weekly quiz as usual.

## Exams:

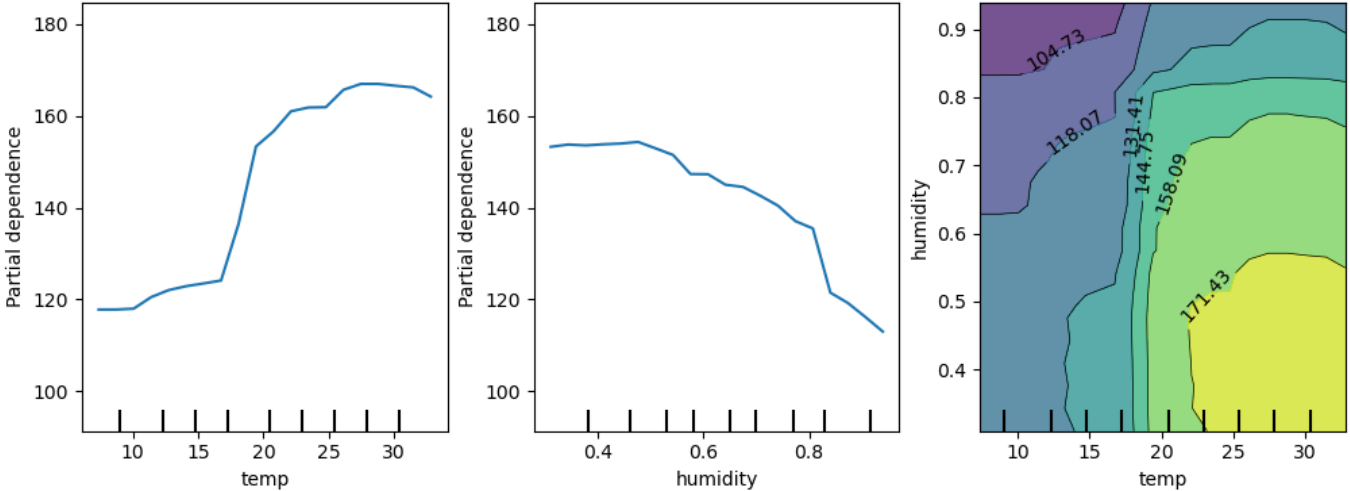
The next exam is on Thursday, 11/21—same format.



# Review

- Model Explainability
  - Partial Difference Plot (PDP)

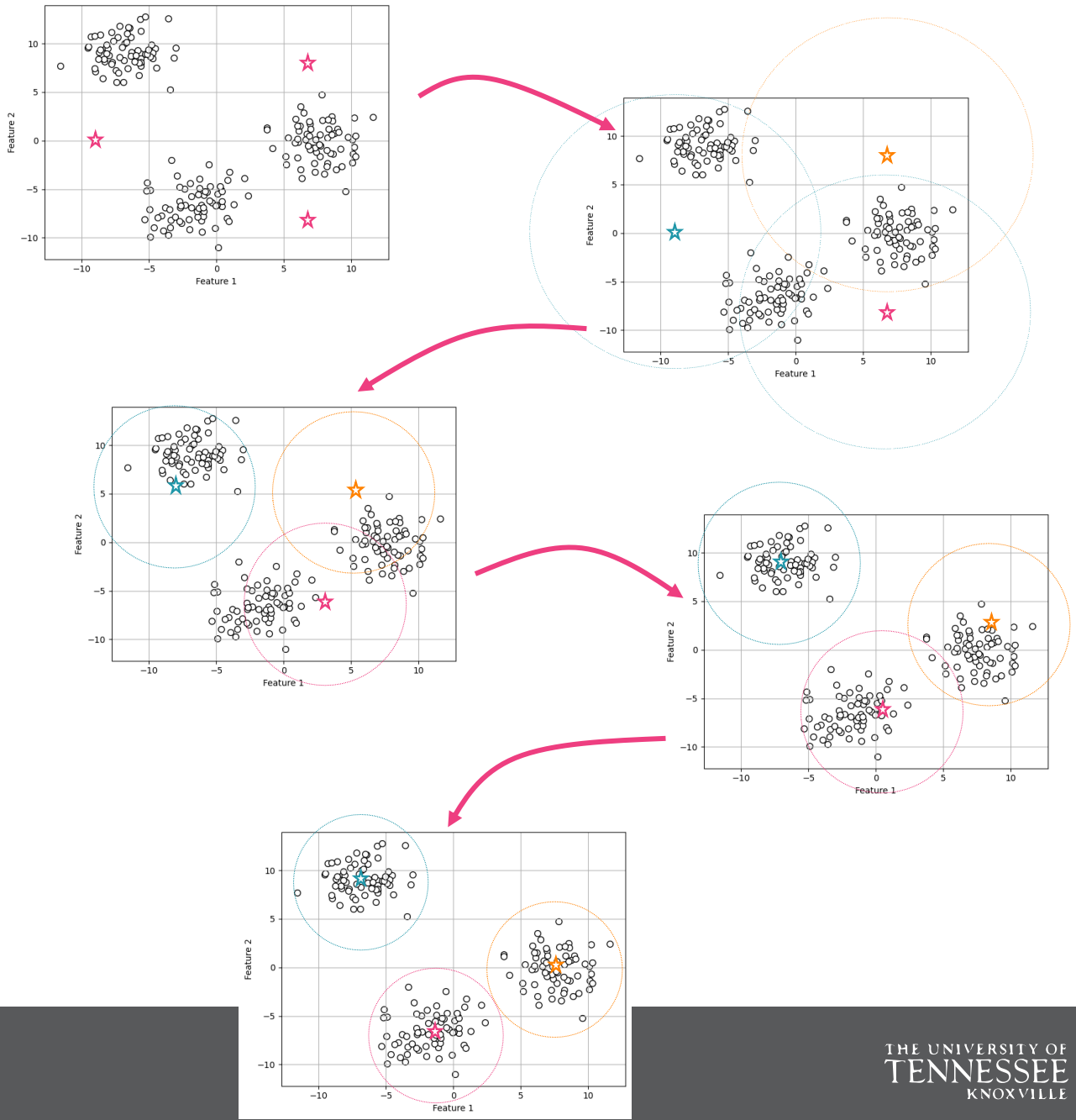
1-way vs 2-way of numerical PDP using gradient boosting





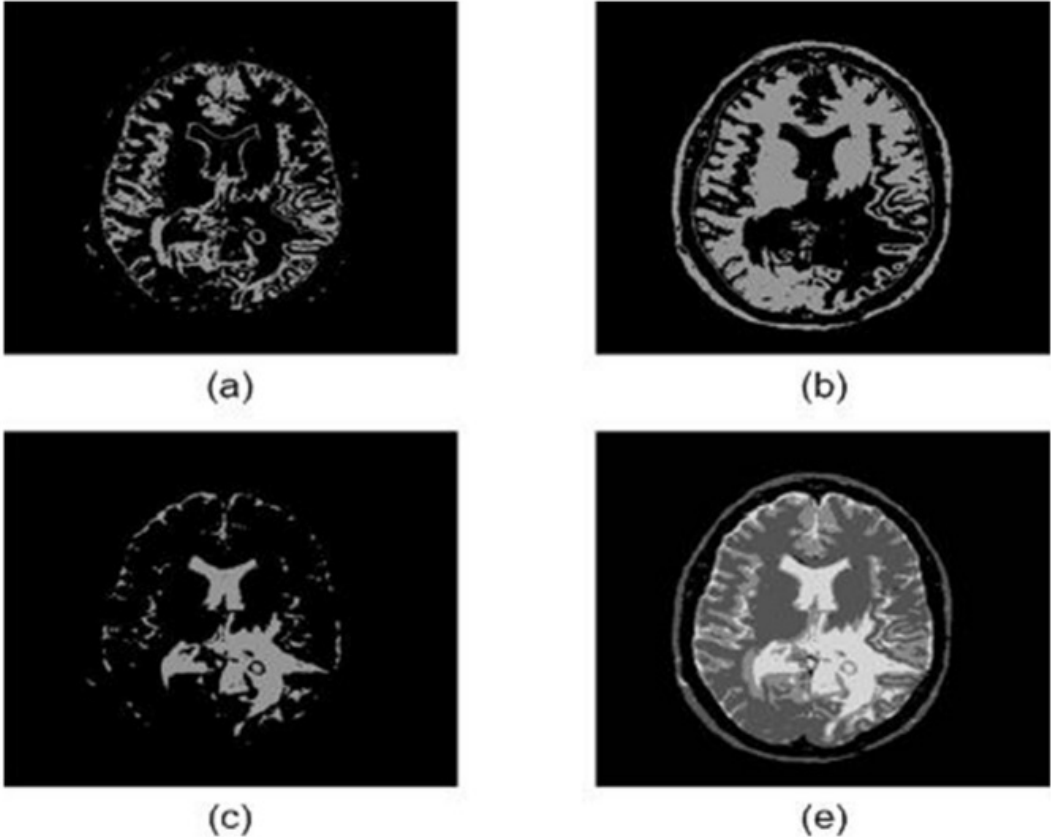
# Review

- Model Explainability
  - Partial Difference Plot (PDP)
- Unsupervised Learning – Clustering algorithms
  - k-means
    - K-means++
    - Elbow method
    - Silhouette analysis



# Review

- Model Explainability
  - Partial Difference Plot (PDP)
- Unsupervised Learning – Clustering algorithms
  - k-means
    - K-means++
    - Elbow method
    - Silhouette analysis
  - Fuzzy-c-means clustering
    - Assigns samples to a cluster and a probability of cluster membership  $[0,1]$  based on the distance of the samples to the cluster's centroid.



FCM Segmentation of (a) Gray Matter, (b) White Matter, (c) Cerebrospinal Fluid, (d) MRI

Dhanachandra and Chanu, "An image segmentation approach based on fuzzy c-means and dynamic particle swarm optimization algorithm," 2020.

Atakishiyev and Reformat, "Analysis of Word Embeddings using Fuzzy Clustering," 2019.

# Review

- Model Explainability
  - Partial Difference Plot (PDP)
- Unsupervised Learning – Clustering algorithms
  - k-means
    - K-means++
    - Elbow method
    - Silhouette analysis
  - Fuzzy-c-means clustering
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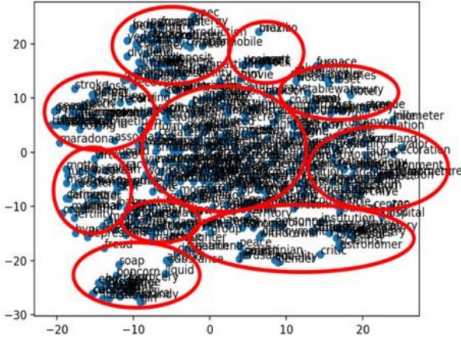


Fig 1. t-SNE Visualization of Word Vectors

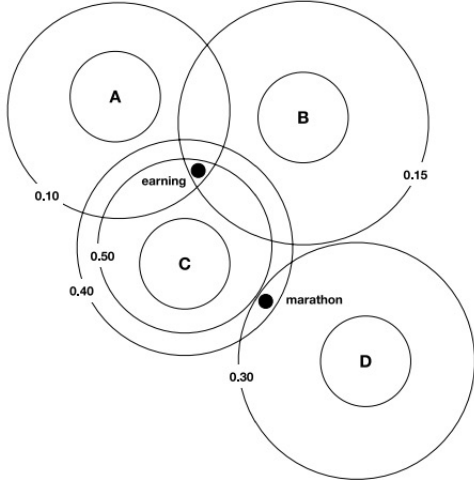


Fig 2. Visualization of words: **earning** and **marathon** that belong to multiple clusters

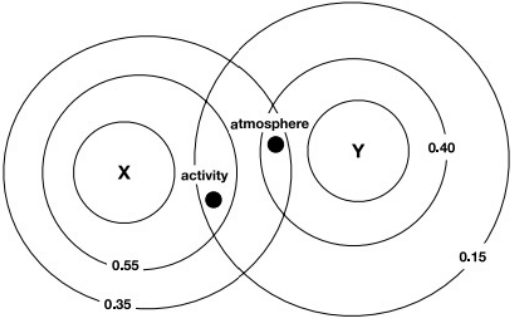


Fig 3. Visualization of words: **activity** and **atmosphere** that belong to two clusters

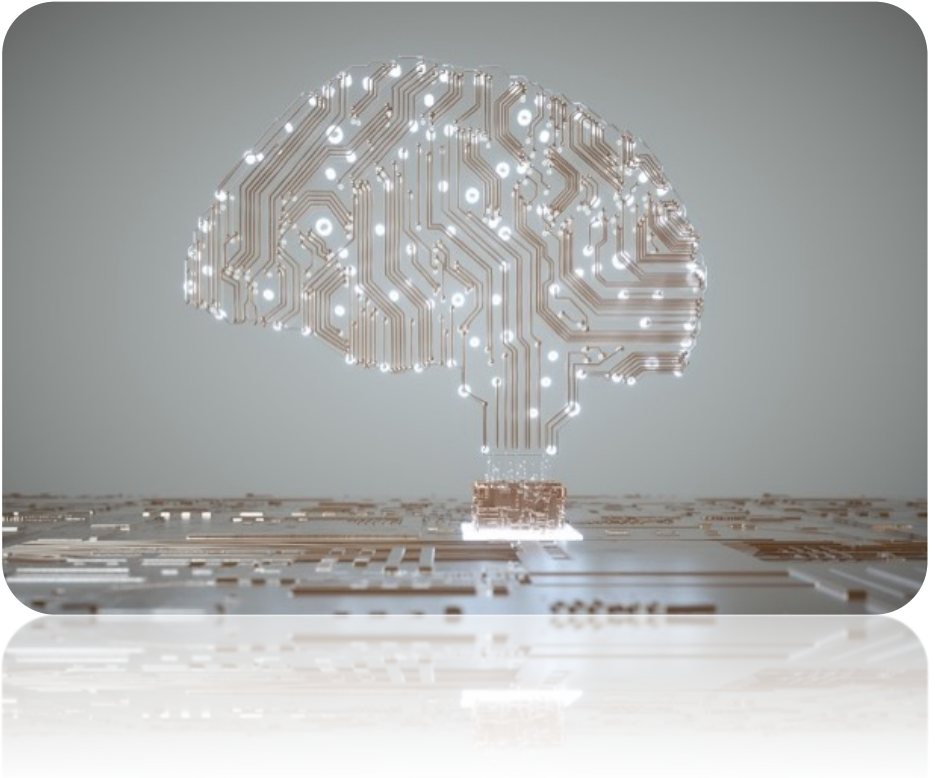


# Today's Topics

*Wrap-up Unsupervised Learning*



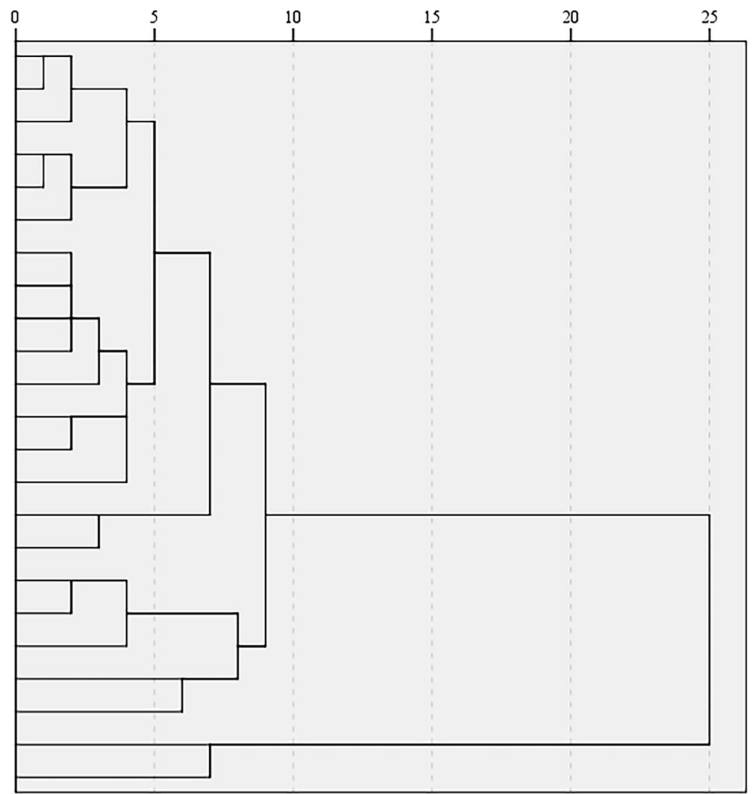
*Neural Networks*



# Hierarchical Clustering

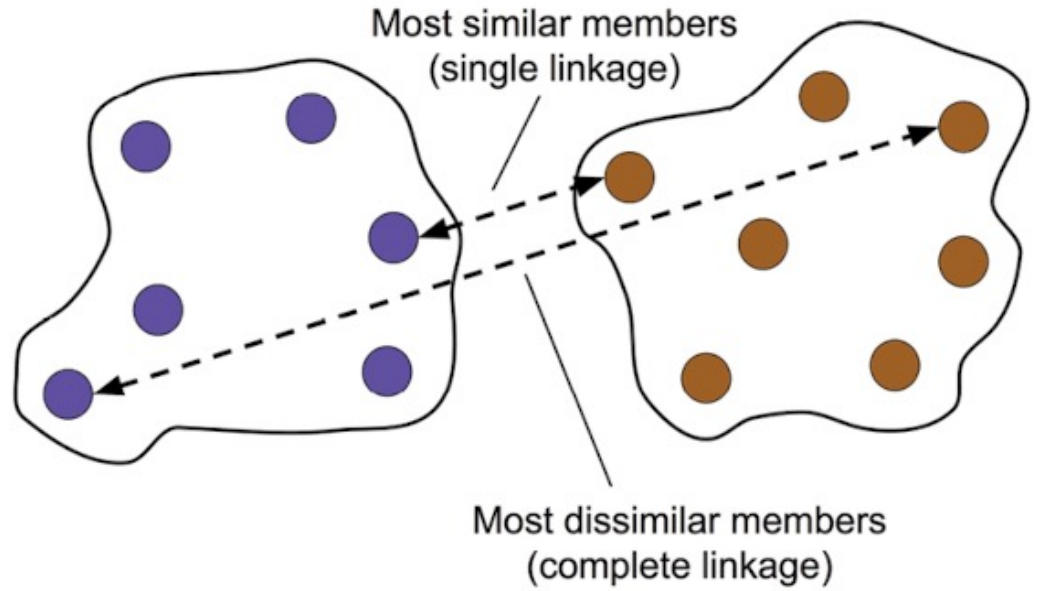
- Bottom-up approach
- Allows plot of dendrograms (Binary hierarchical clustering)
- No need to specify the number of clusters  $k$
- Two main approaches
  - Divisive method:
    - The whole dataset belongs to a single cluster
    - Split cluster
    - Stop when each sample is a cluster
  - **Agglomerative method:**
    - Starts with each sample as a cluster
    - Merge clusters until all samples belong to a single cluster

*Dendrogram example*



# Agglomerative Method

- Single linkage
  - Compares the most similar samples
- **Complete linkage**
  - Compares the most different samples



Raschka, et. al., "Machine Learning with PyTorch and Scikit-Learn: Develop machine learning and deep learning models with Python"

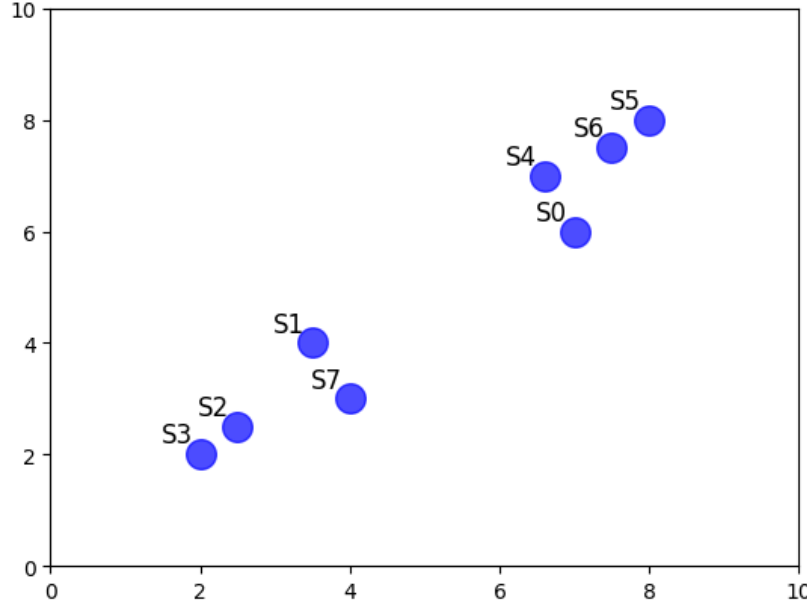


# Agglomerative Complete Linkage Algorithm

1. Compute a pair-wise distance matrix of all samples.
2. Represent each data point as a singleton cluster.
3. Merge the two closest clusters based on the distance between the ***most dissimilar (distant) members***.
4. Update the cluster linkage matrix.
5. Repeat steps 2-4 until one single cluster remains.

# Step-by-Step Example

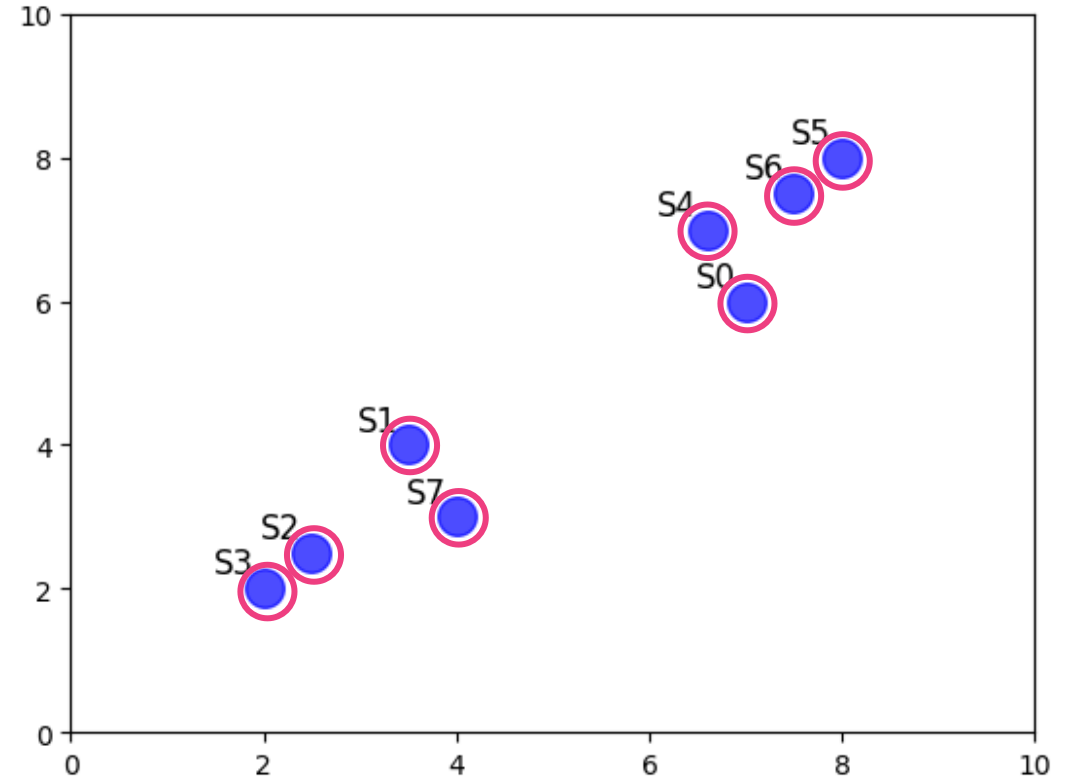
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	S0	S1	S2	S3	S4	S5	S6	S7
S0	0.0	4.0	5.7	6.4	1.1	2.2	1.6	4.2
S1	4.0	0.0	1.8	2.5	4.3	6.0	5.3	1.1
S2	5.7	1.8	0.0	0.7	6.1	7.8	7.1	1.6
S3	6.4	2.5	0.7	0.0	6.8	8.5	7.8	2.2
S4	1.1	4.3	6.1	6.8	0.0	1.7	1.0	4.8
S5	2.2	6.0	7.8	8.5	1.7	0.0	0.7	6.4
S6	1.6	5.3	7.1	7.8	1.0	0.7	0.0	5.7
S7	4.2	1.1	1.6	2.2	4.8	6.4	5.7	0.0

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1. Compute a pair-wise distance matrix of all samples.
2. **Represent each data point as a singleton cluster.**
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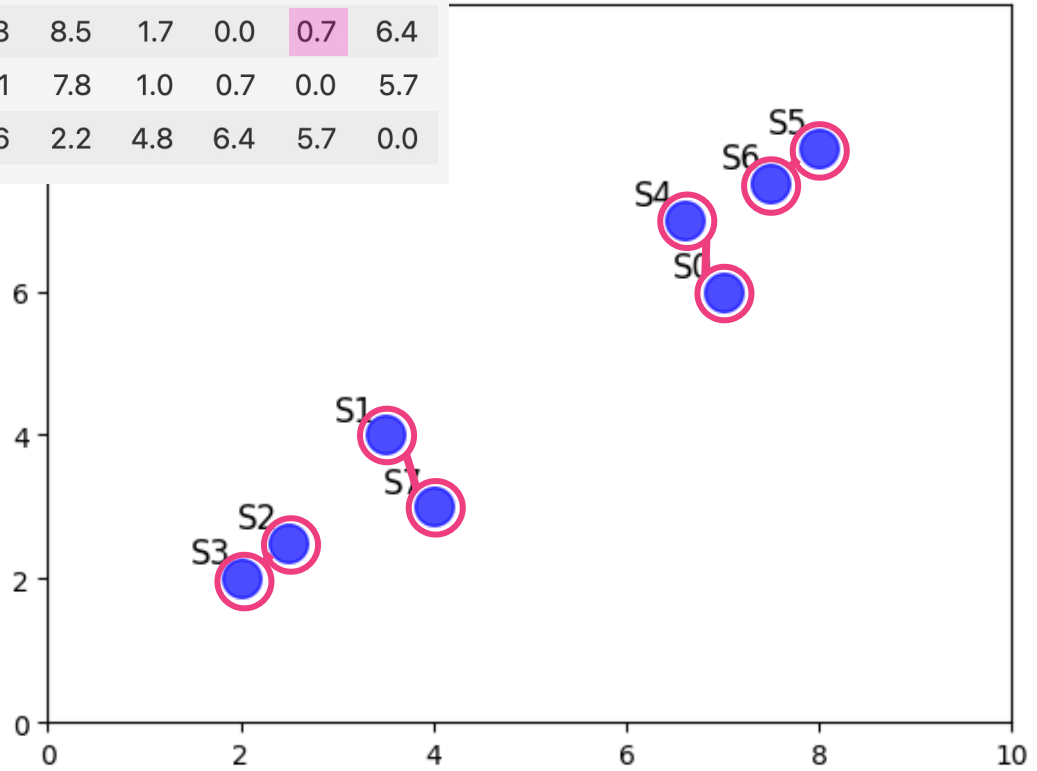




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S4	1.1	4.3	6.1	6.8	0.0	1.7	1.0	4.8
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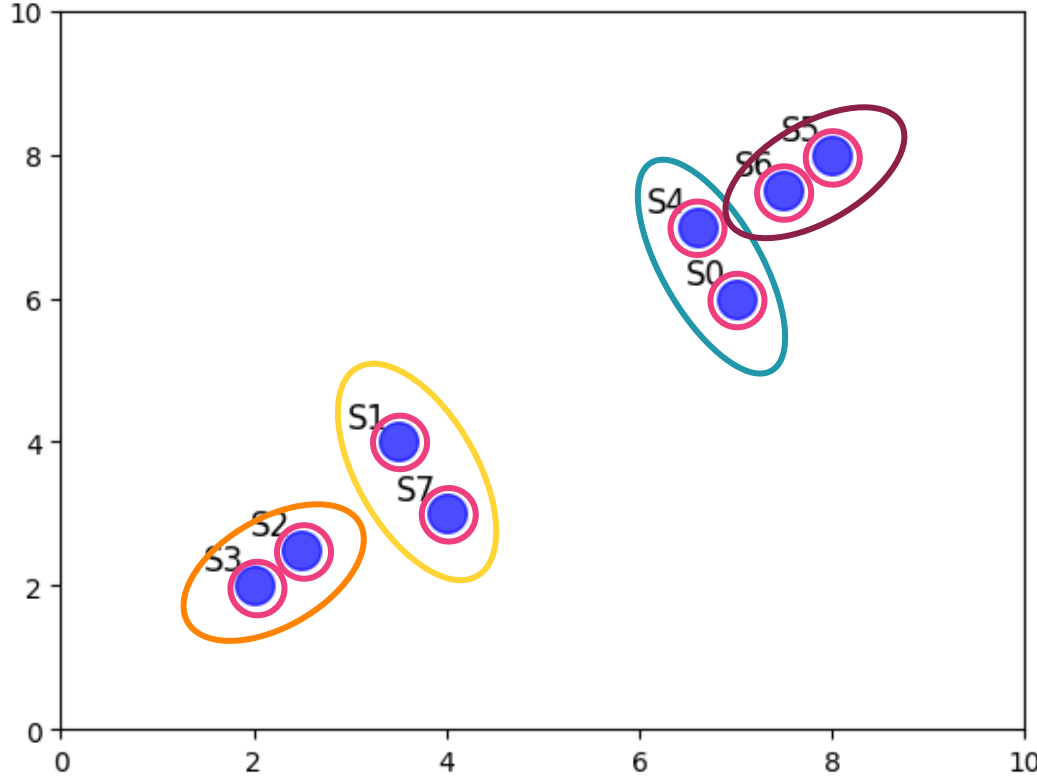
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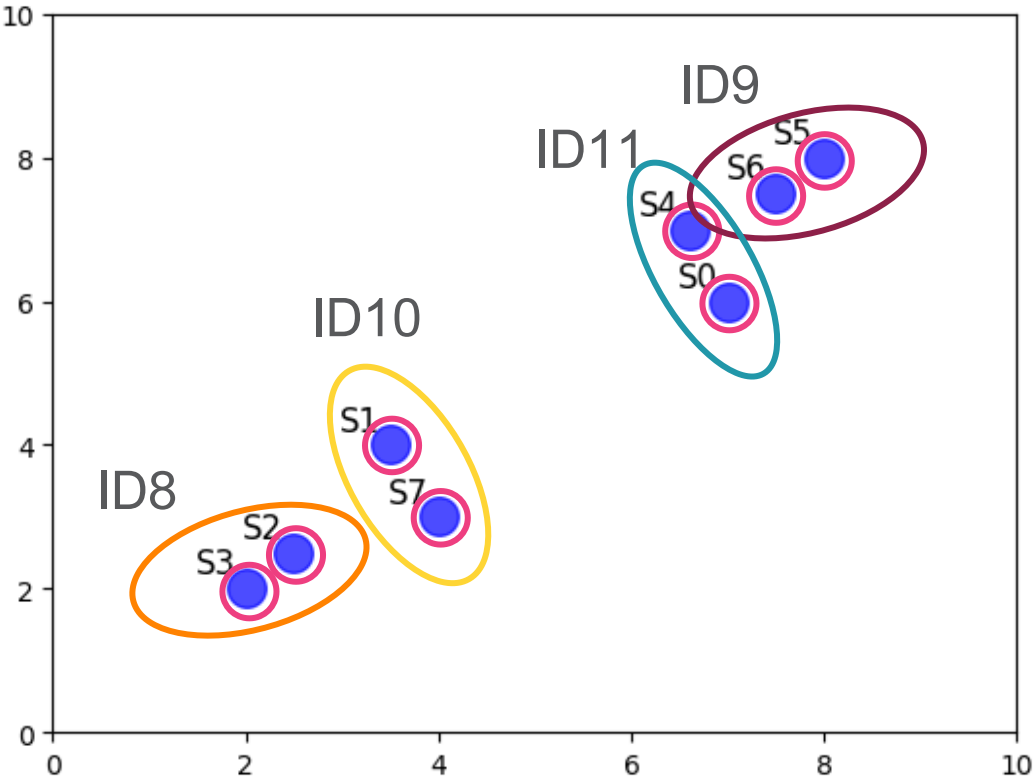
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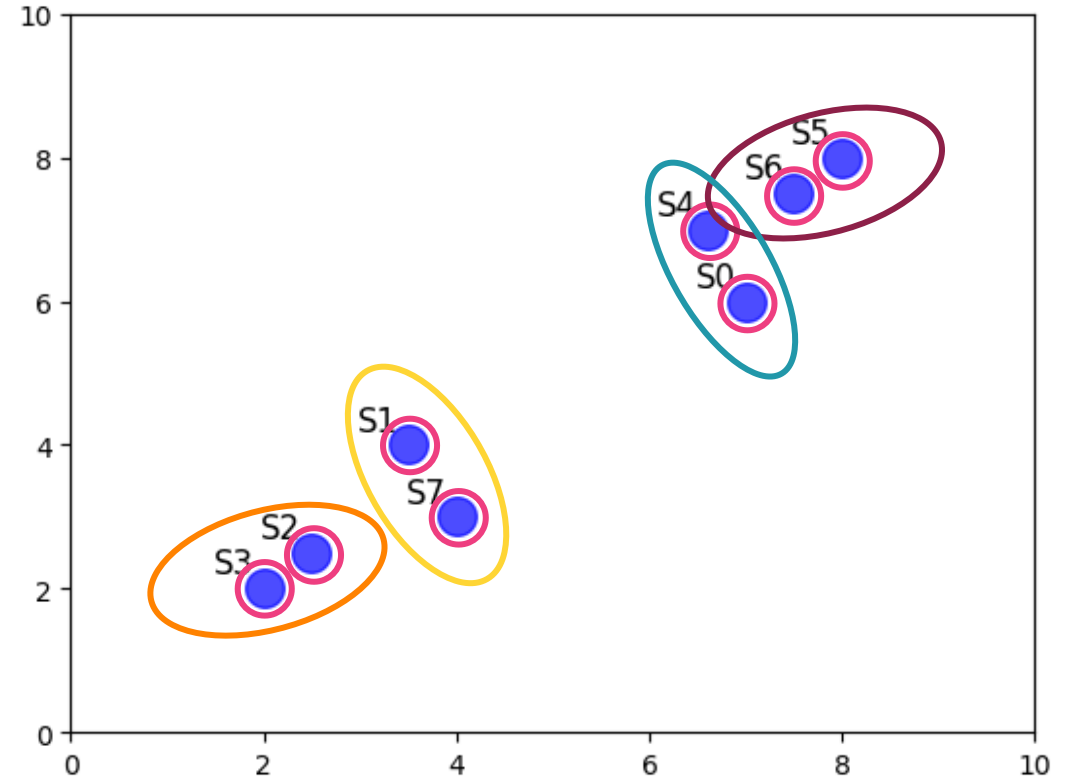
# Linkage Matrix Update

Cluster	Label 1	Label 2	Distance	# of samples
Cluster 8	2	3	0.7	2
Cluster 9	5	6	0.7	2
Cluster 10	1	7	1.1	2
Cluster 11	0	4	1.1	2



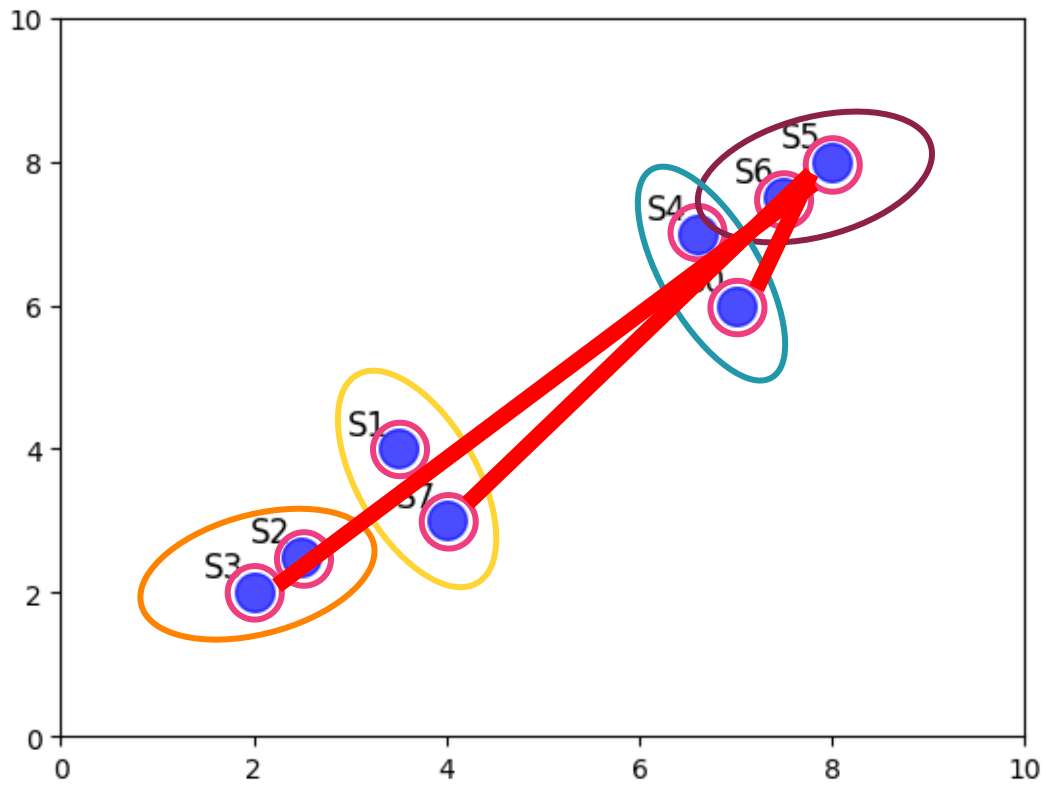
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# Step-by-Step Example

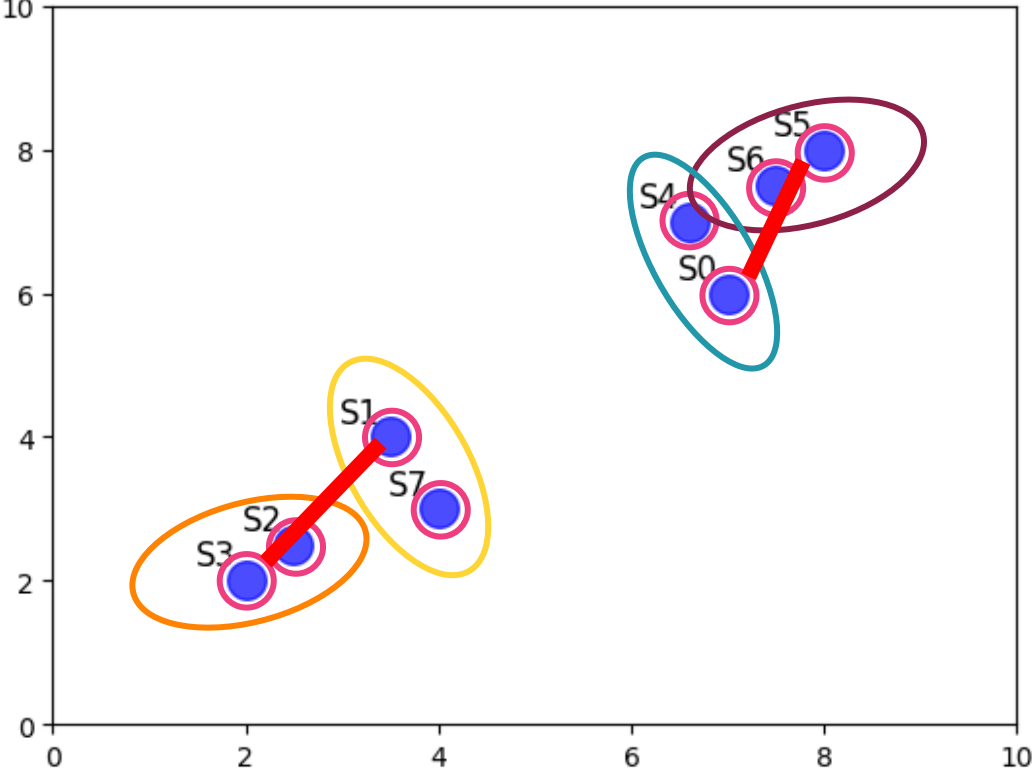
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S4	1.1	4.3	6.1	6.8	0.0	1.7	1.0	4.8
S5	2.2	6.0	7.8	8.5	1.7	0.0	0.7	6.4
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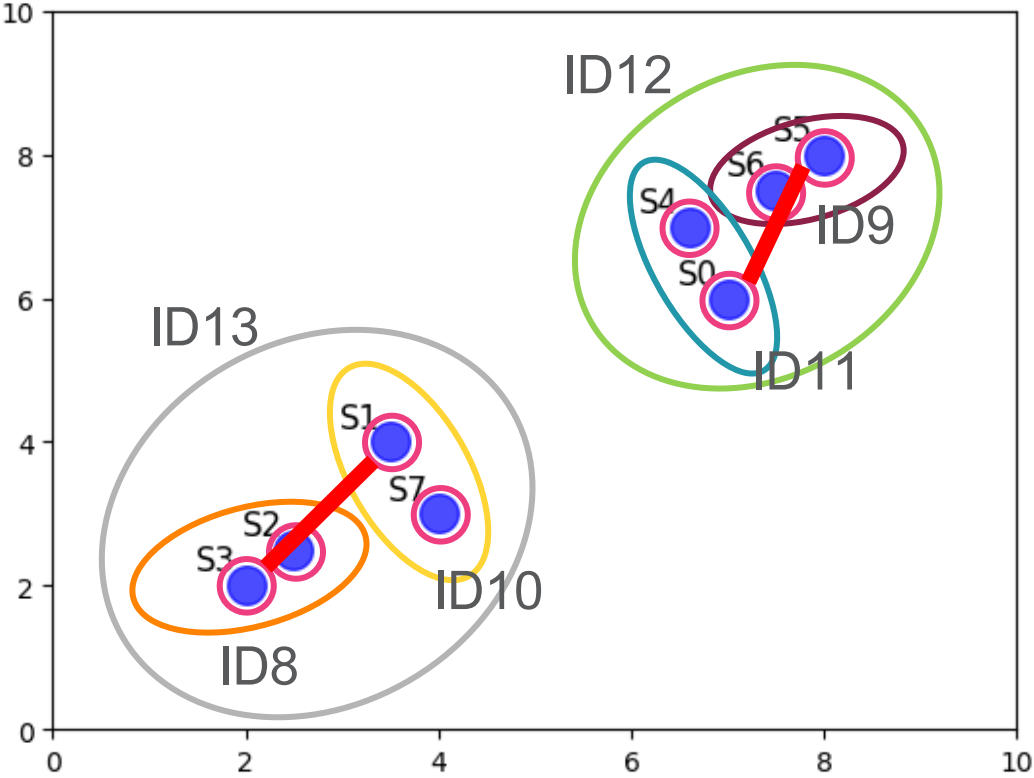
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S3	6.4	2.5	0.7	0.0	6.8	8.5	7.8	2.2
S4	1.1	4.3	6.1	6.8	0.0	1.7	1.0	4.8
S5	2.2	6.0	7.8	8.5	1.7	0.0	0.7	6.4
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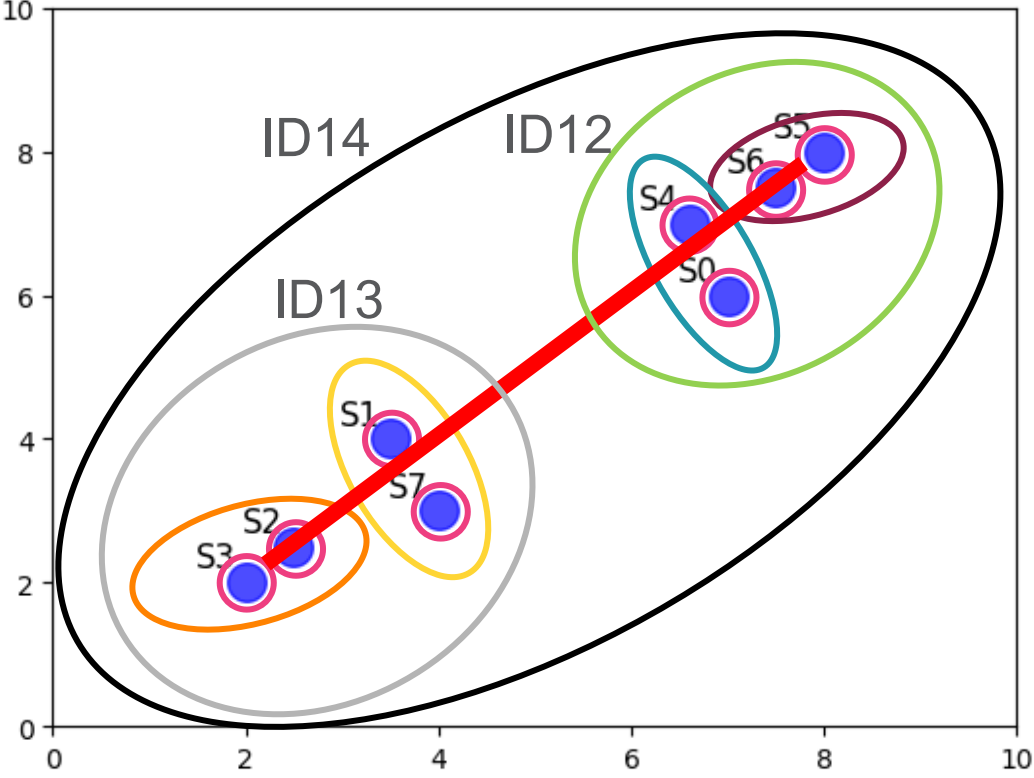
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Cluster 12	9	11	2.2	4
Cluster 13	8	10	2.5	4



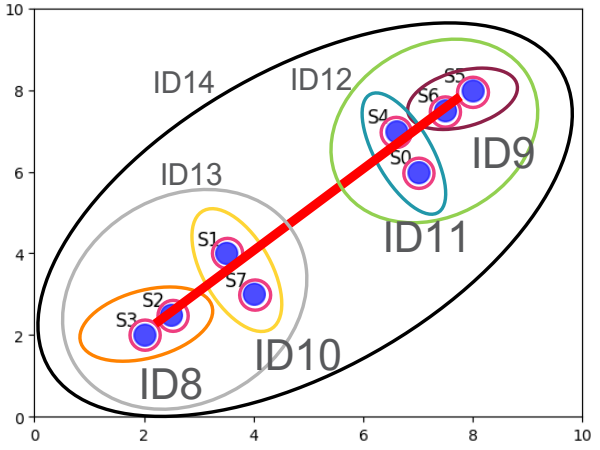
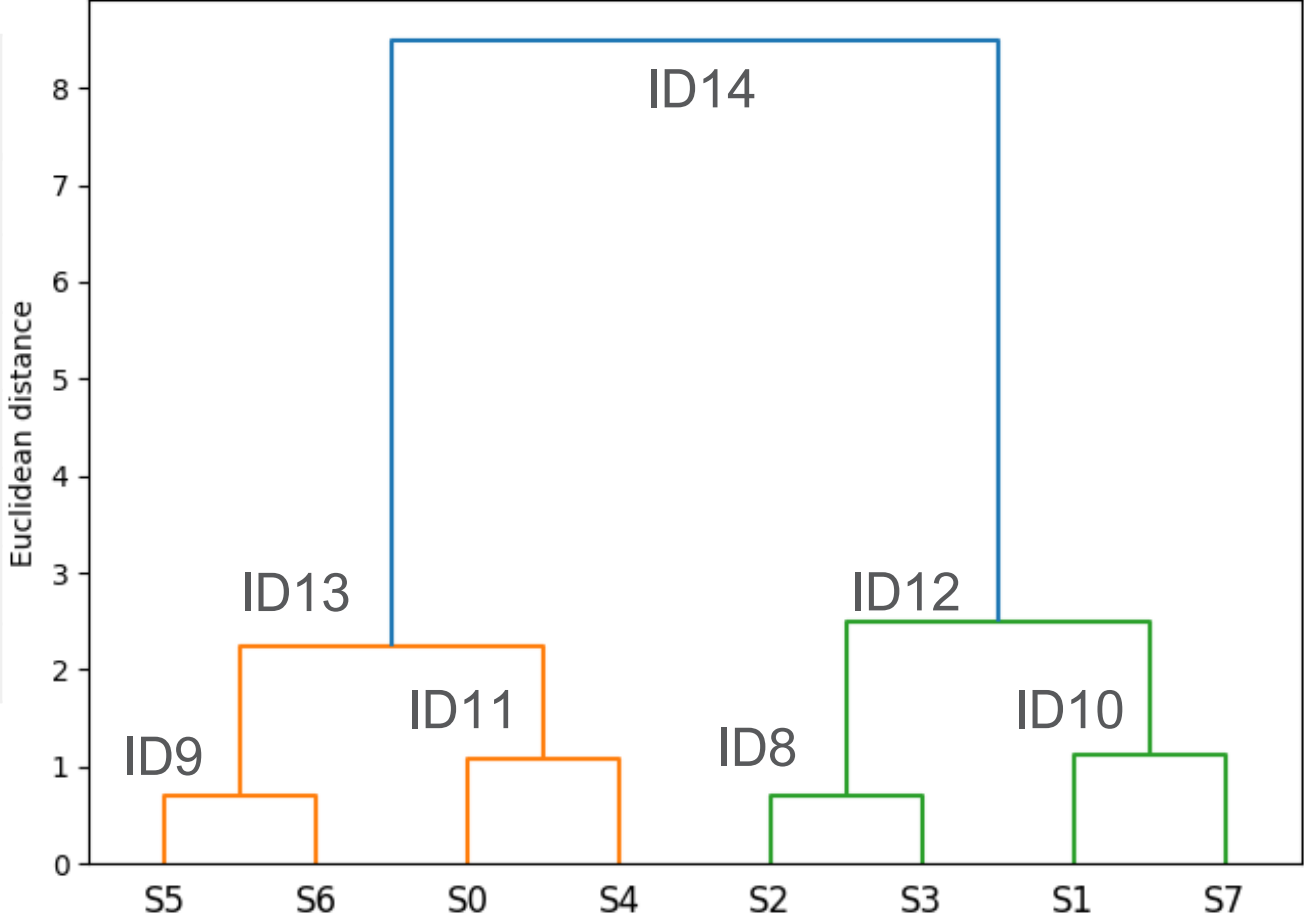
# Linkage Matrix Update: Final Step

Cluster	Label 1	Label 2	Distance	# of samples
Cluster 8	2	3	0.7	2
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Cluster 12	9	11	2.2	4
Cluster 13	8	10	2.5	4
Cluster 14	12	13	8.5	8



# Dendrogram

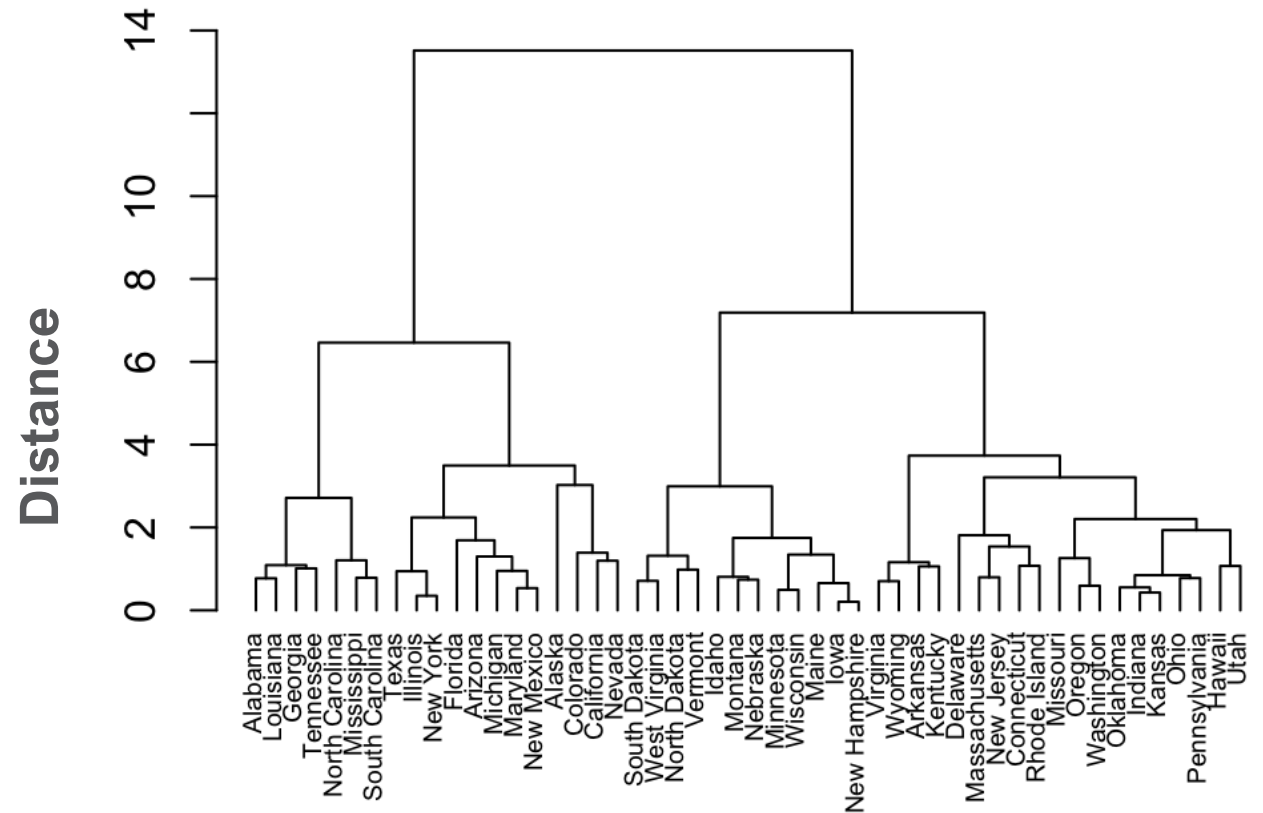
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# Dendrogram

- Hierarchical relationship
- Selecting the number of clusters
- Similarity between clusters
- Identifying outliers
- Cluster stability
  - Multiple runs

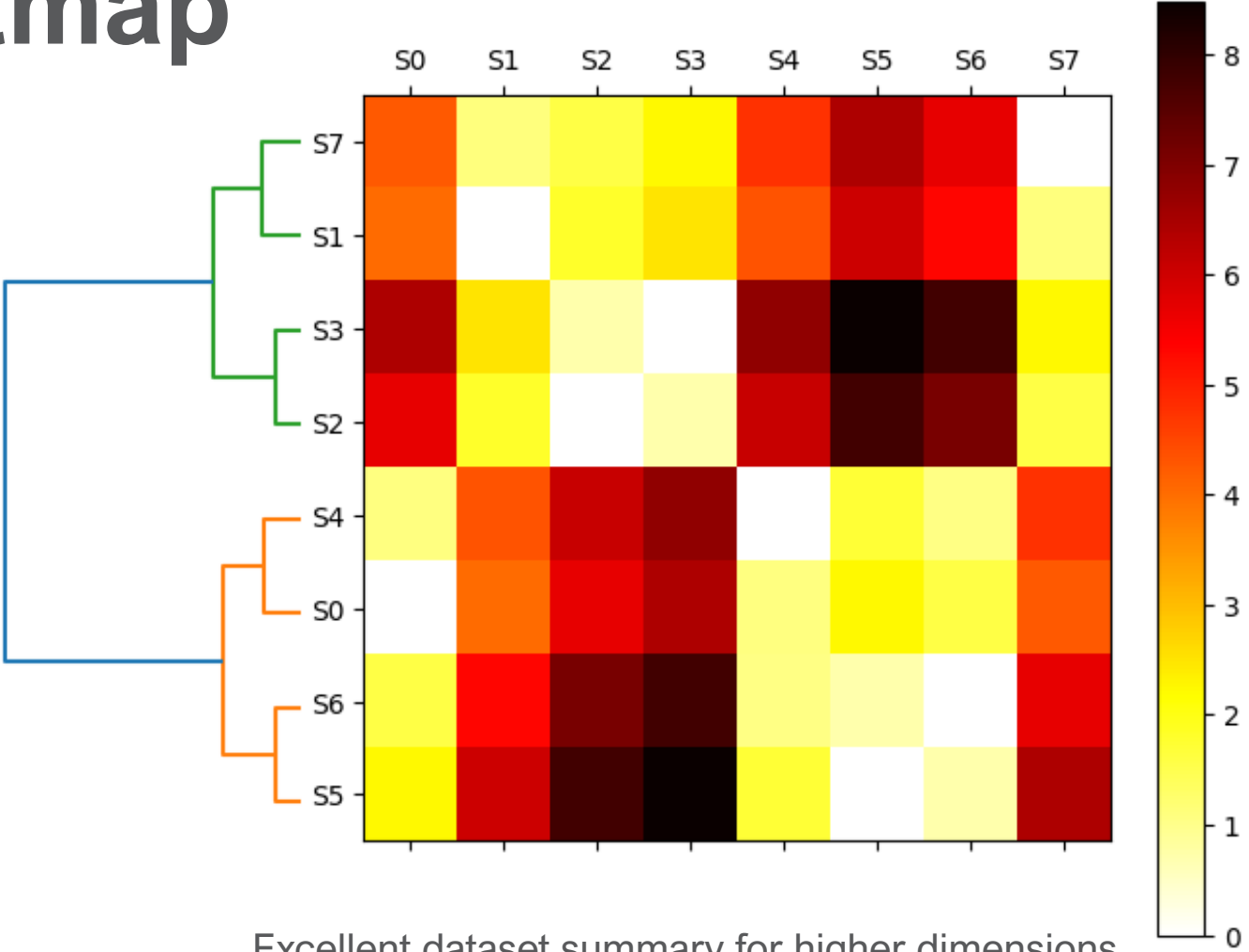
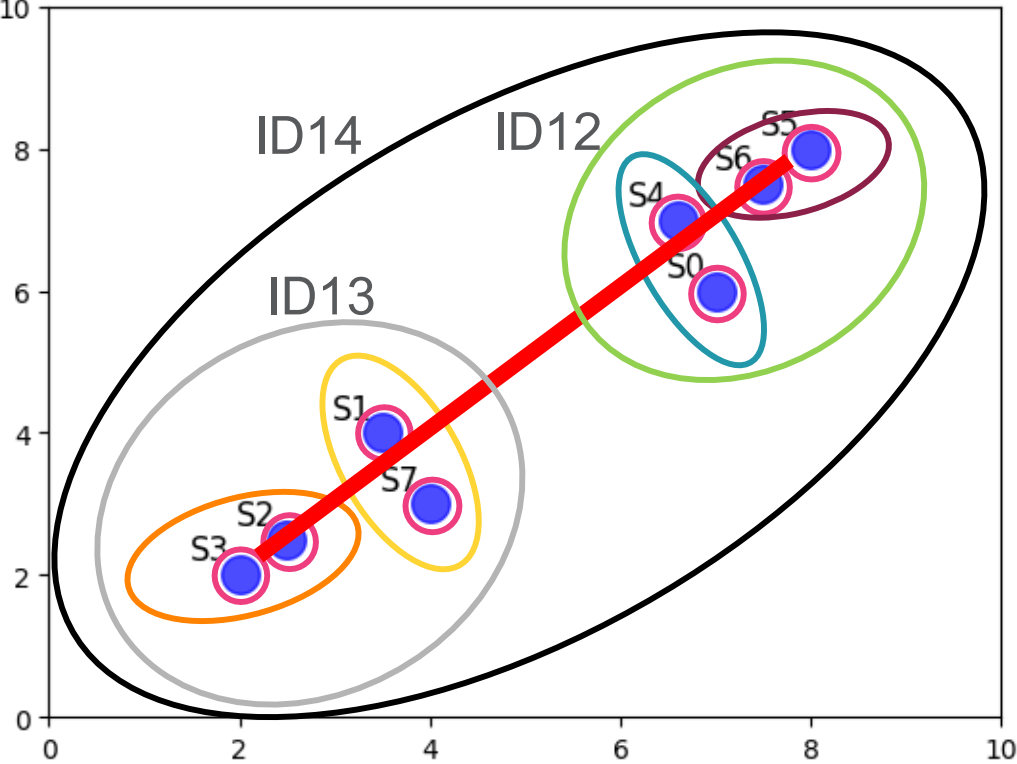
## USA Arrests Cluster Dendrogram



<https://www.kaggle.com/datasets/halimedogan/usarrests>



# Dendrogram + Heatmap

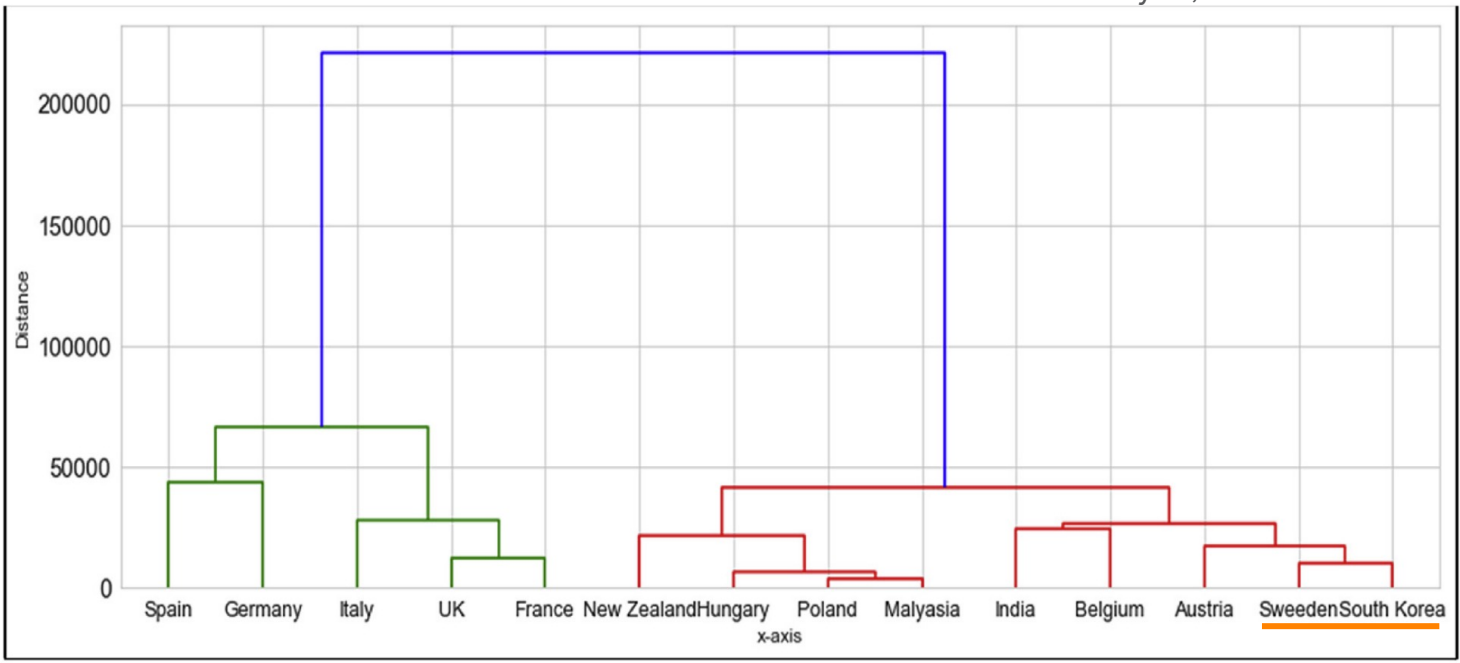


Excellent dataset summary for higher dimensions

# Applications of Hierarchical Clustering

- Customer segmentation
- Image segmentation
- Anomaly detection
- Recommendation systems
- Document retrieval
- Market Segmentation

Gosal, et. al., "Impact of complete lockdown on total infection and death rates: A hierarchical cluster analysis," 2020.



**Fig. 4.** Hierarchical clustering of death rates of the 17 countries (15 with lockdown & 2 without lockdown divided into two clusters). X-axis: countries; Y-axis: distance from the mean. Cluster 1: Spain, Germany, Italy, UK, and France. Cluster: Belgium, Austria, New Zealand, India, Hungary, Poland, Malaysia, Sweden and South Korea. Blue lines: Division of the two main clusters. Green lines: Individual countries under cluster 1. Red lines: Individual countries under cluster 2.

# Pop Quiz

True or False. A dendrogram visualizes the correlations between data features.

A. True

B. False





# Artificial Neural Networks



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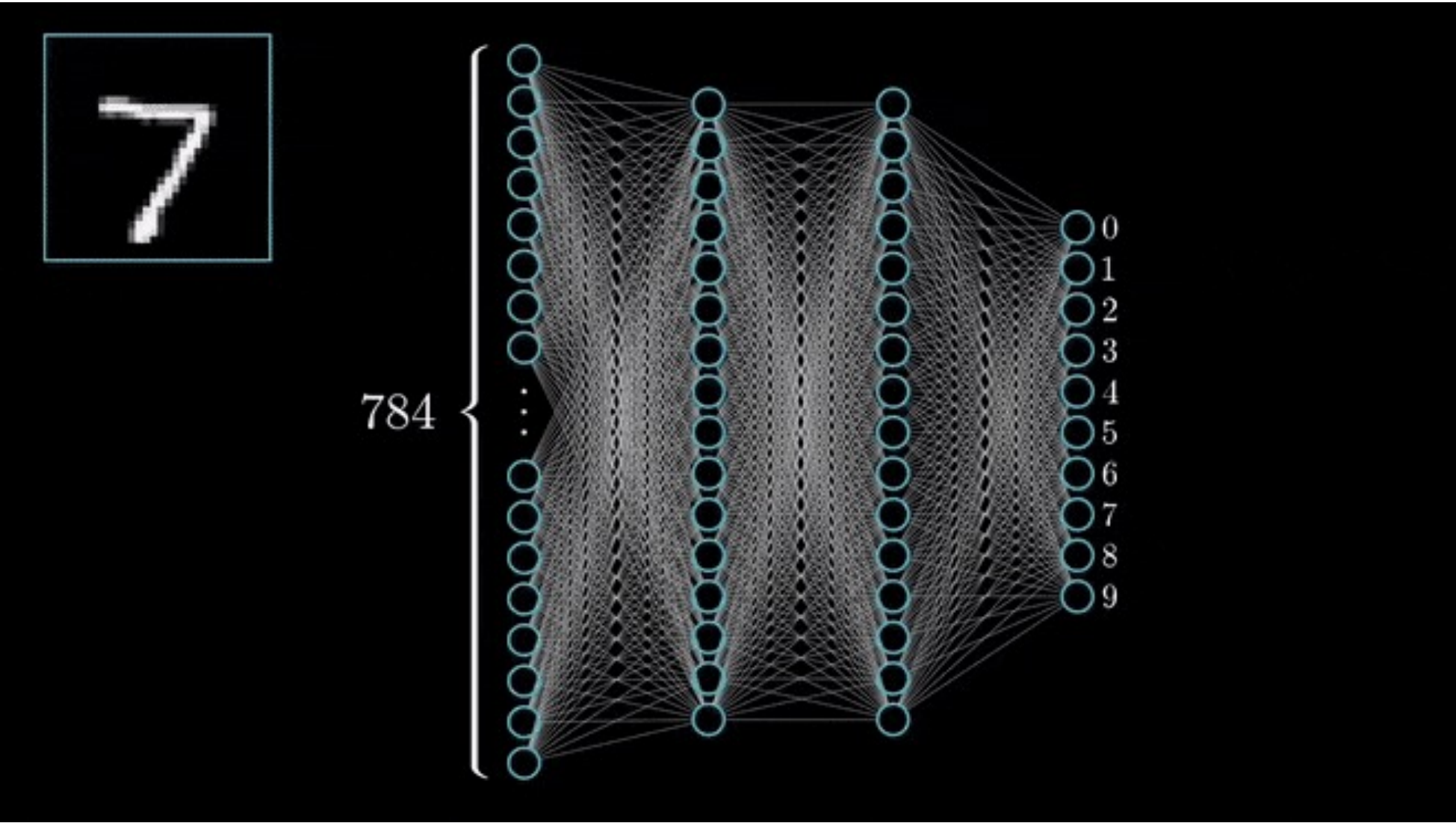




**For a deep dive into ANNs and Deep Learning**

COSC 425/524 this Spring

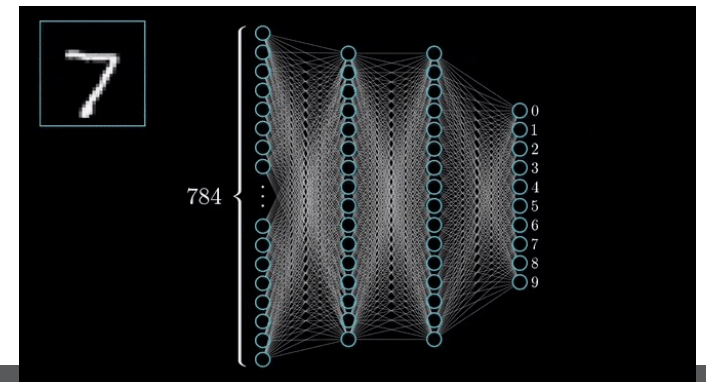




# Why does it work?

The short answers:

1. Universal approximation theorem – Any continuous function can be represented using a ***feed-forward neural network*** (does not discuss how to learn)
2. The ***backpropagation algorithm*** is an efficient way to learn the weights in a feedforward network.



# Logistic Regression

- Linear regression:  $\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_m x_m = X\theta$

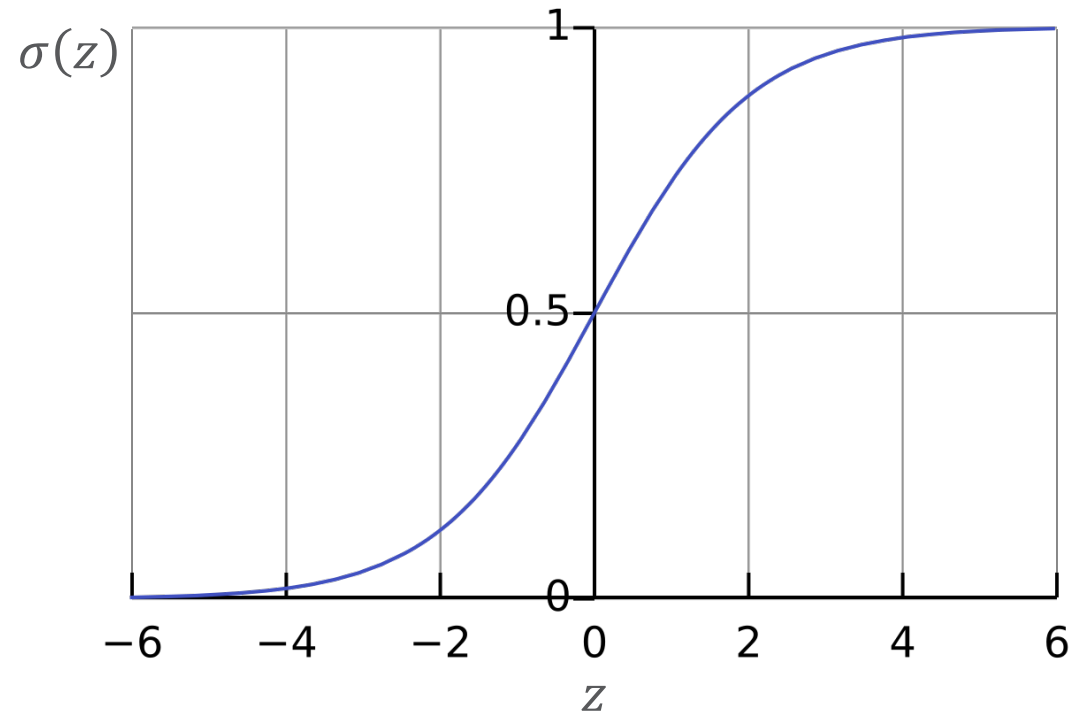
- Logistic regression:

- $z = X\theta$

- $\hat{p} = \sigma(z)$

- $\sigma(z) = \frac{1}{1+e^{-z}} \Rightarrow \hat{p} = \frac{1}{1+e^{-X\theta}}$

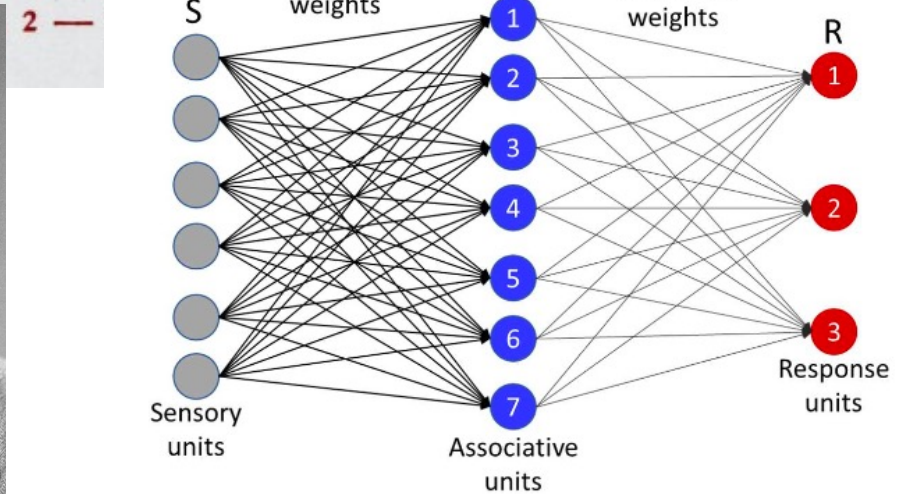
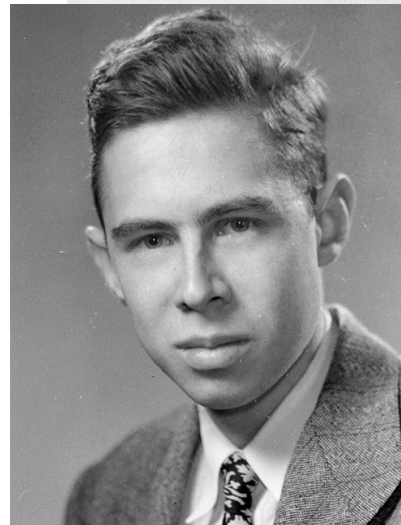
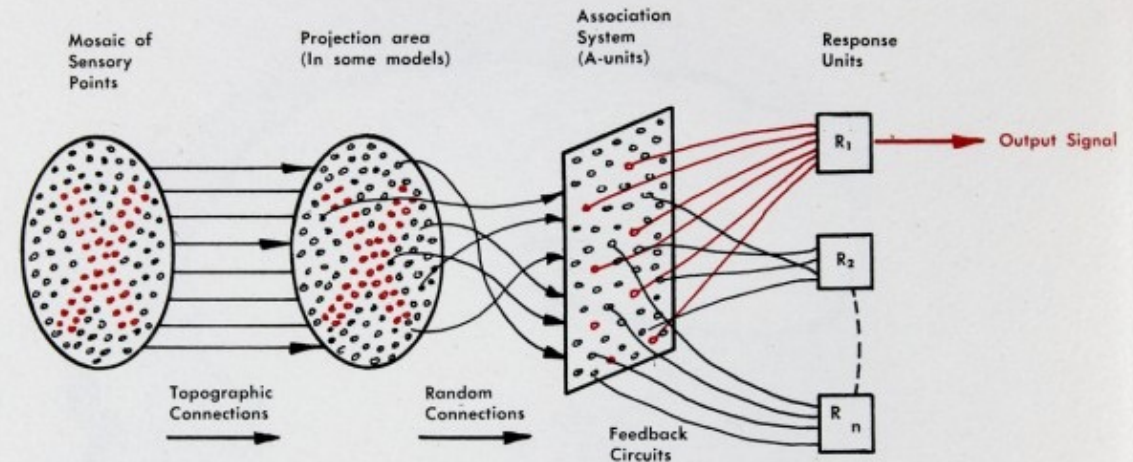
- $\hat{y} = \begin{cases} 1, & \hat{p} \geq 0.5 \\ 0, & \hat{p} < 0.5 \end{cases}$



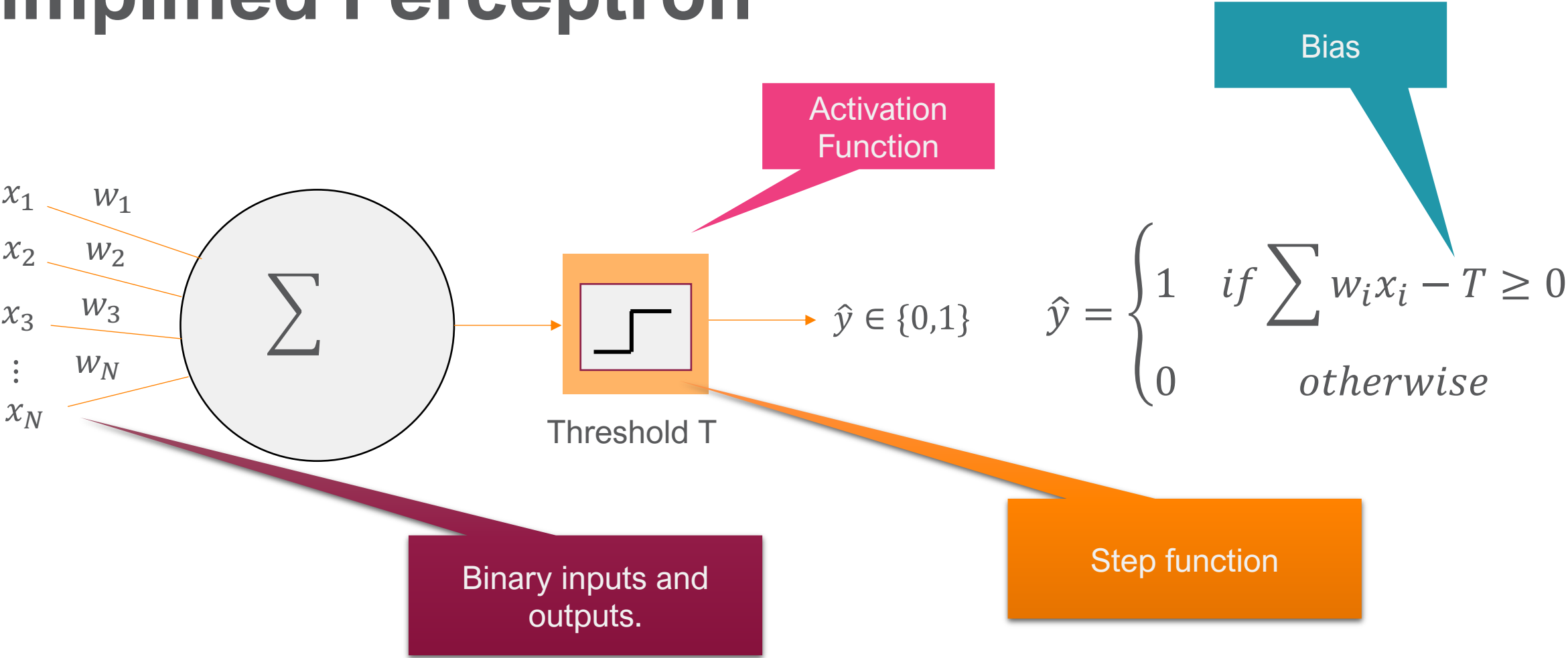
# Rosenblatt's Mark I: The Perceptron

- Frank Rosenblatt was a psychologist and logician
- Inventor of the perceptron in 1957 with the paper "The Perceptron—a perceiving and recognizing automaton"
- Funded by the U.S. Office of Naval Research
- Inspired by McCulloch-Pitts (MCP) neuron

**FIG. 1 — Organization of a biological brain.** (Red areas indicate active cells, responding to the letter X.)

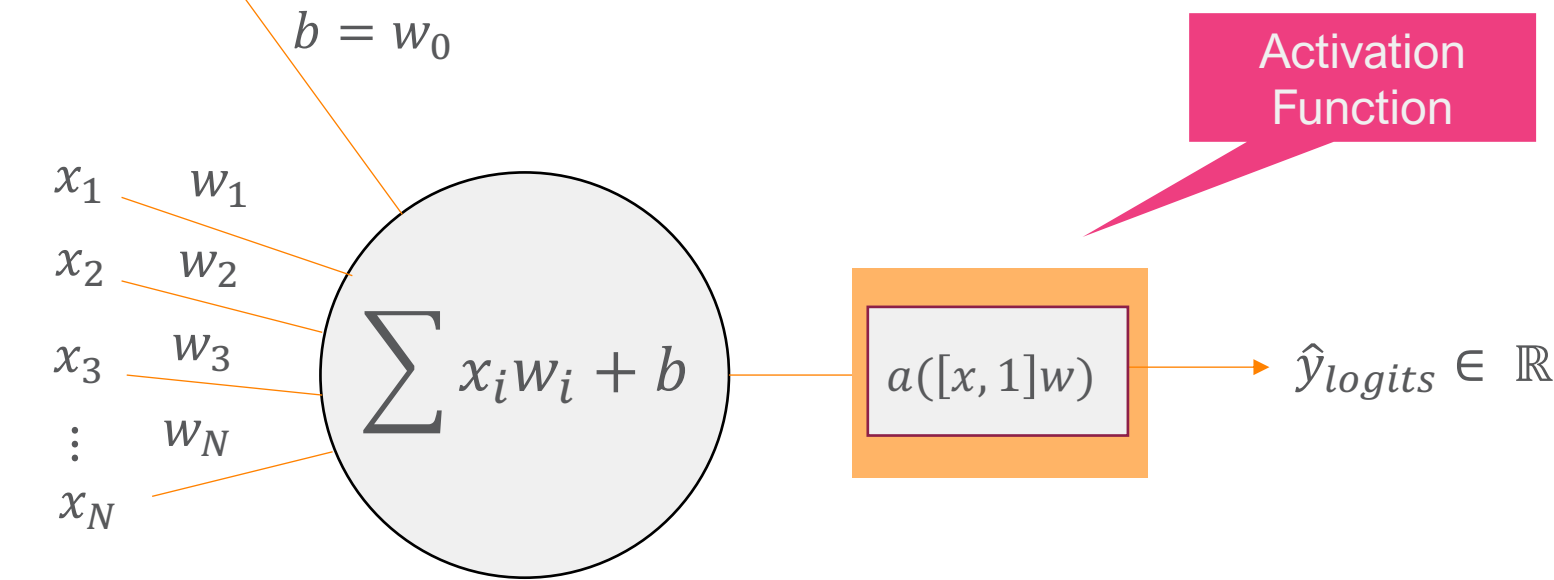


# Simplified Perceptron





# Modern Perceptron



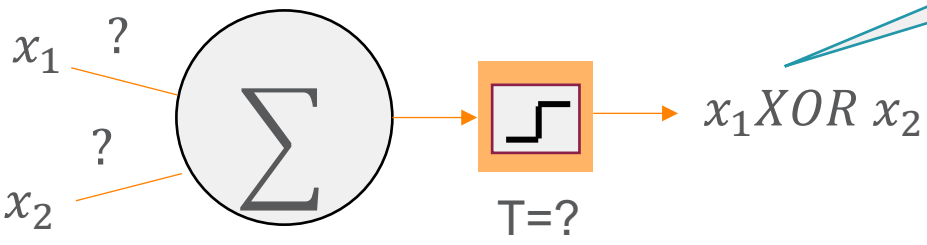
$$\hat{y} = \begin{cases} 1 & \text{if } \hat{y}_{logits} \geq T \\ 0 & \text{otherwise} \end{cases}$$

$x_i \in \mathbb{R} \quad w_i \in \mathbb{R}$

Real inputs and outputs.

# Limitations

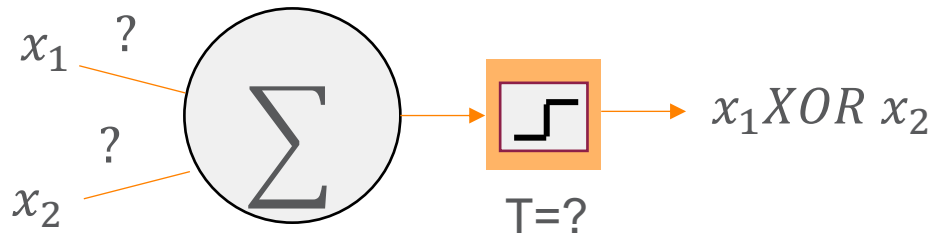
- Still, binary inputs and outputs



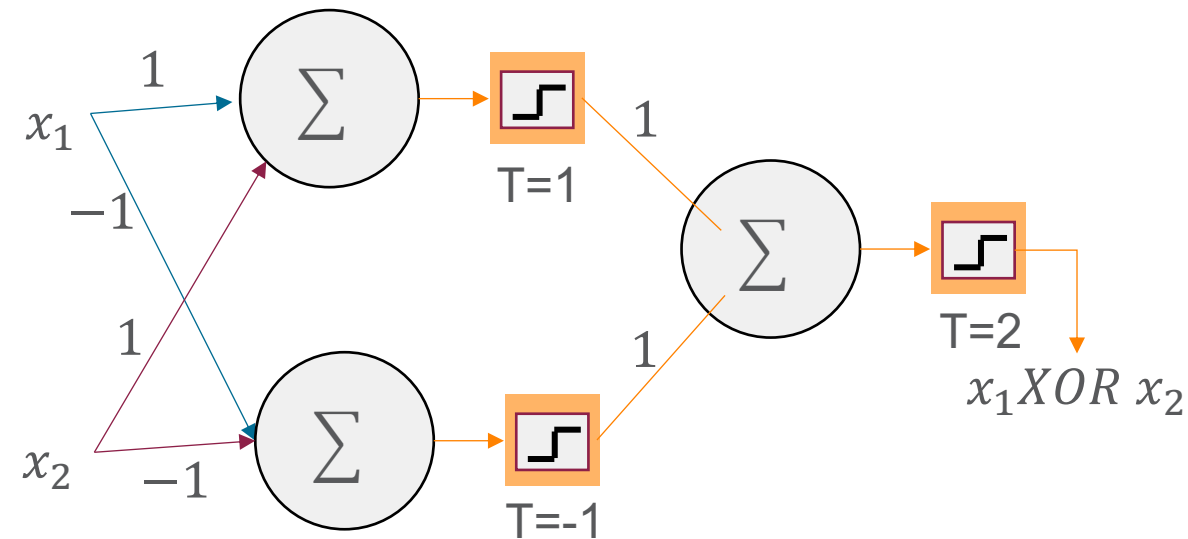
*Can we compute XOR?*

# Limitations

- Still, binary inputs and outputs
- No solution for XOR or non-linear functions

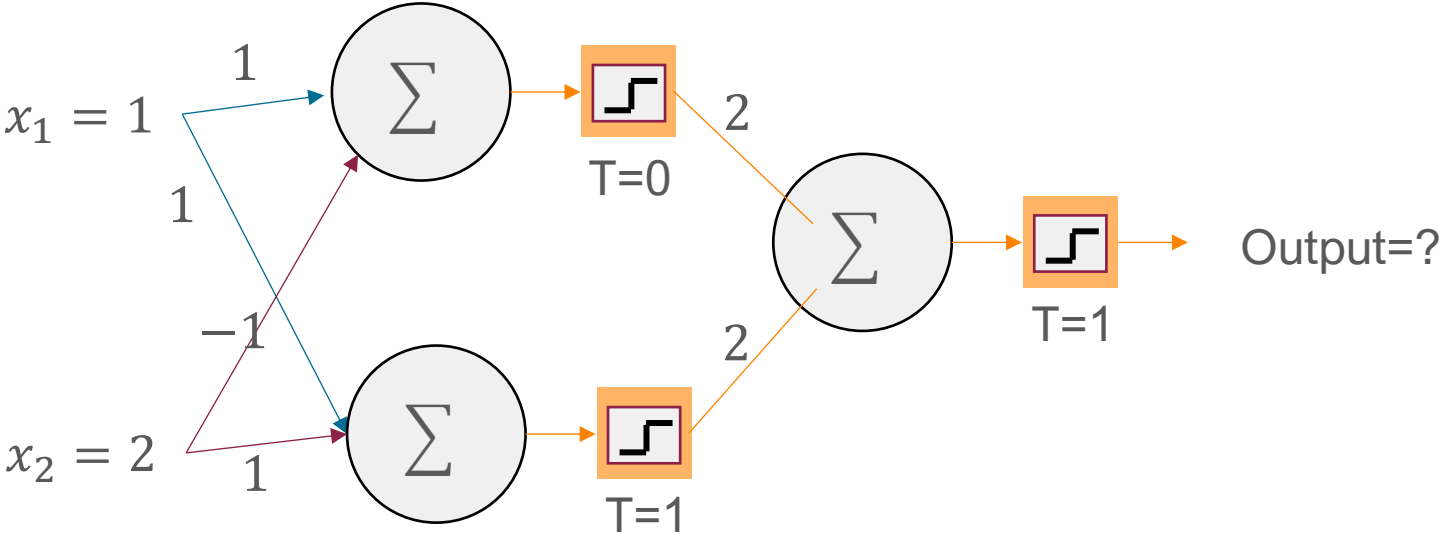


## Solution: Multi-layer Perceptron



More on MLP soon.

# Pop Quiz

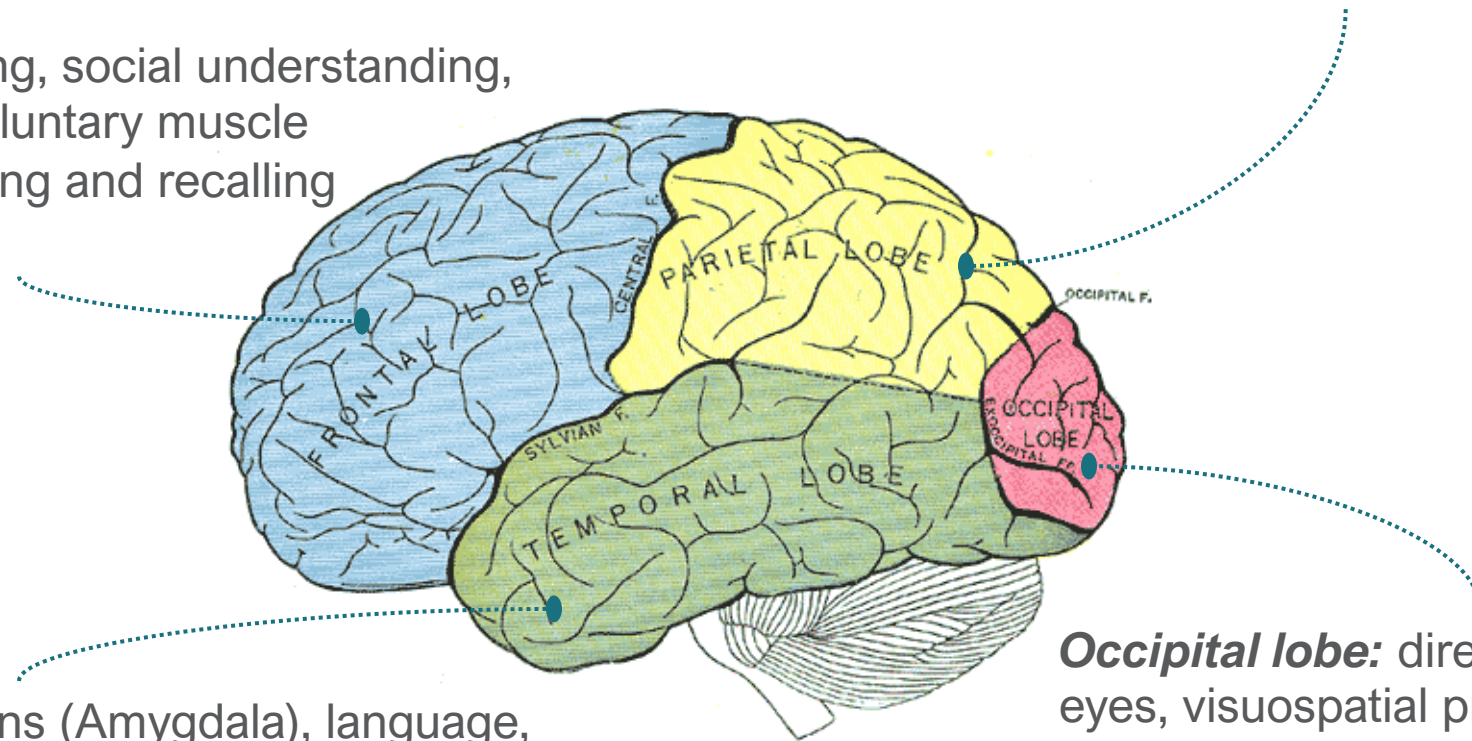


- A. Output=-1
- B. Output=0
- C. Output=1
- D. Output=2

# Human Brain

**Parietal lobe:** Integrates the brain processes, writing, self-perception, location awareness, and touch senses such as pressure, heat, cold, vibrations, and pain.

**Frontal lobe:** Reasoning, social understanding, executive functions, voluntary muscle movements, and learning and recalling information.

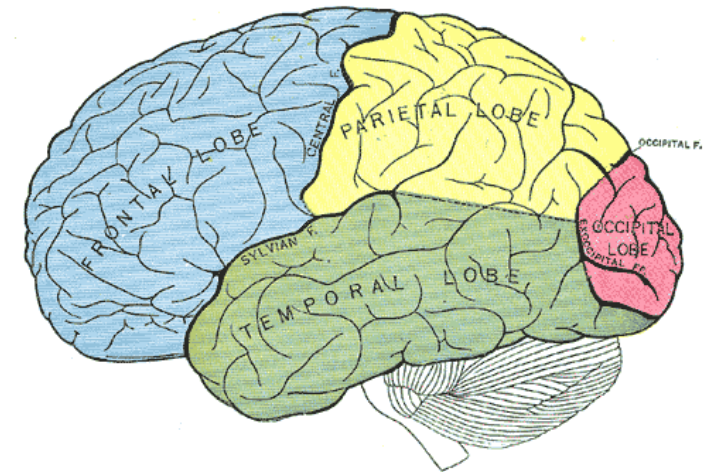
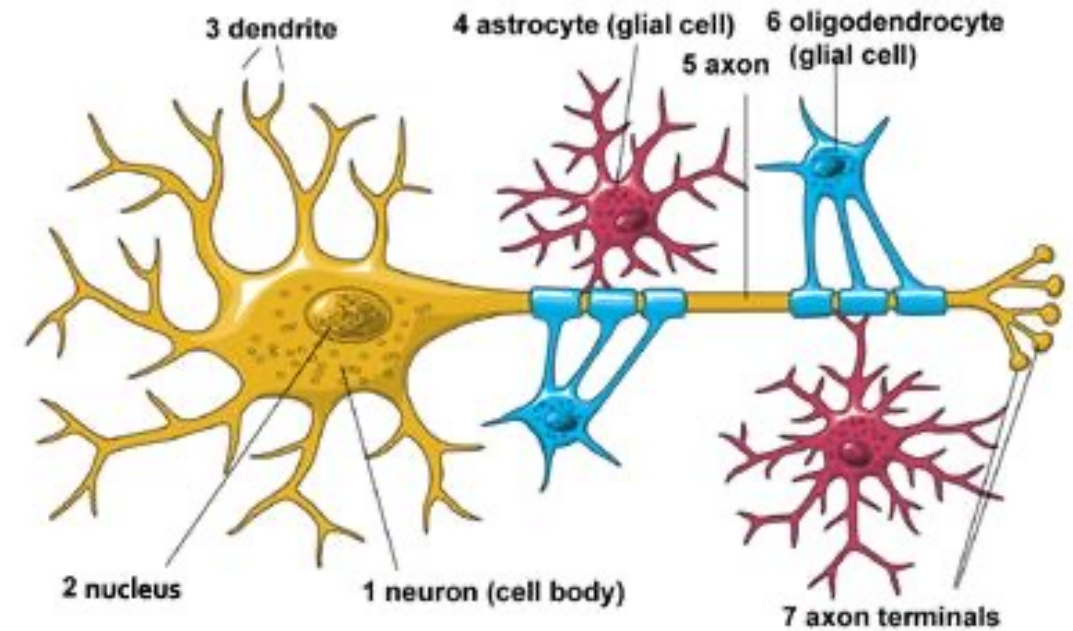


**Temporal lobe:** Emotions (Amygdala), language, memory (hippocampus), sight and sound processing, and object recognition.

**Occipital lobe:** direct connection to the eyes, visuospatial processing, distance and depth perception, color determination, object and face recognition.

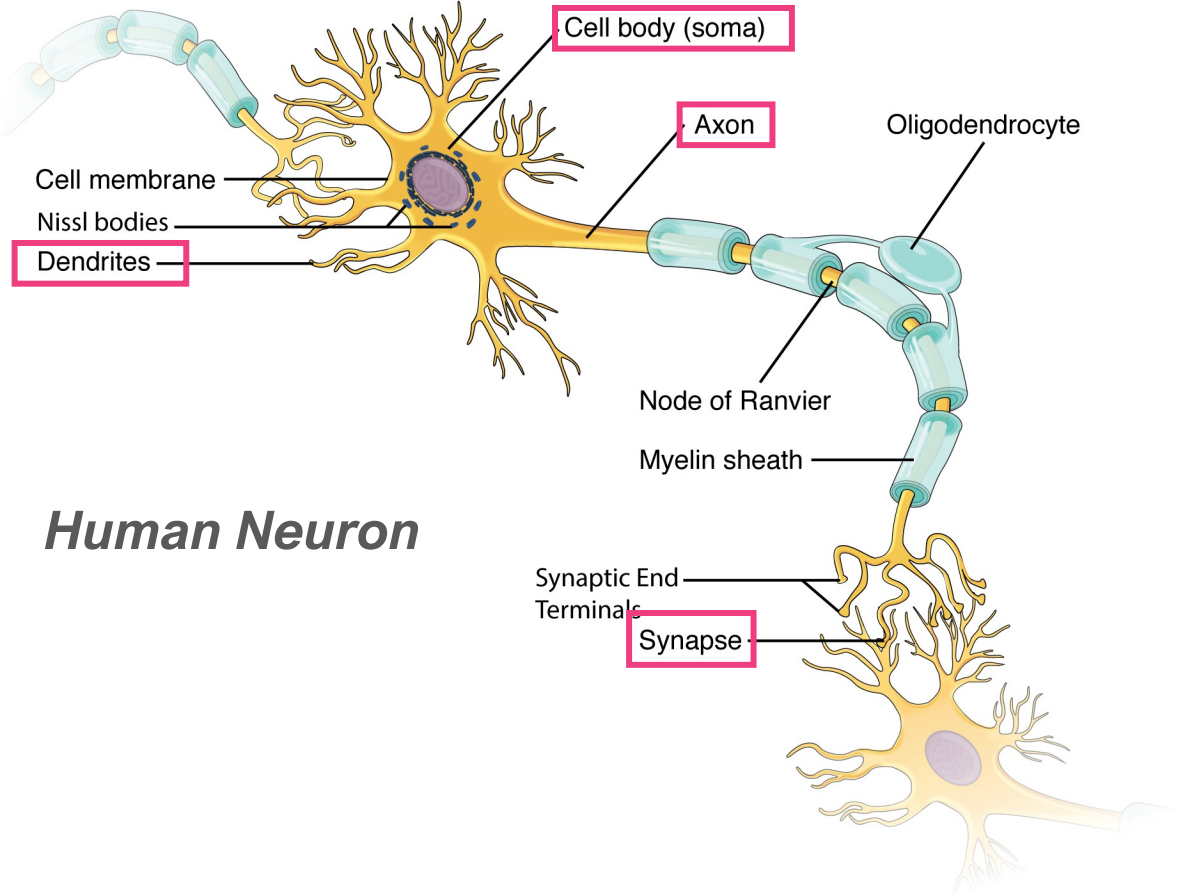
# A neuron

- Dendrites – receive signals from other neurons
- Soma (Cell Body) – Process information received from dendrites
- Axon – Transmit the output of the Soma
- Synapses – Small connections between axon and dendrites

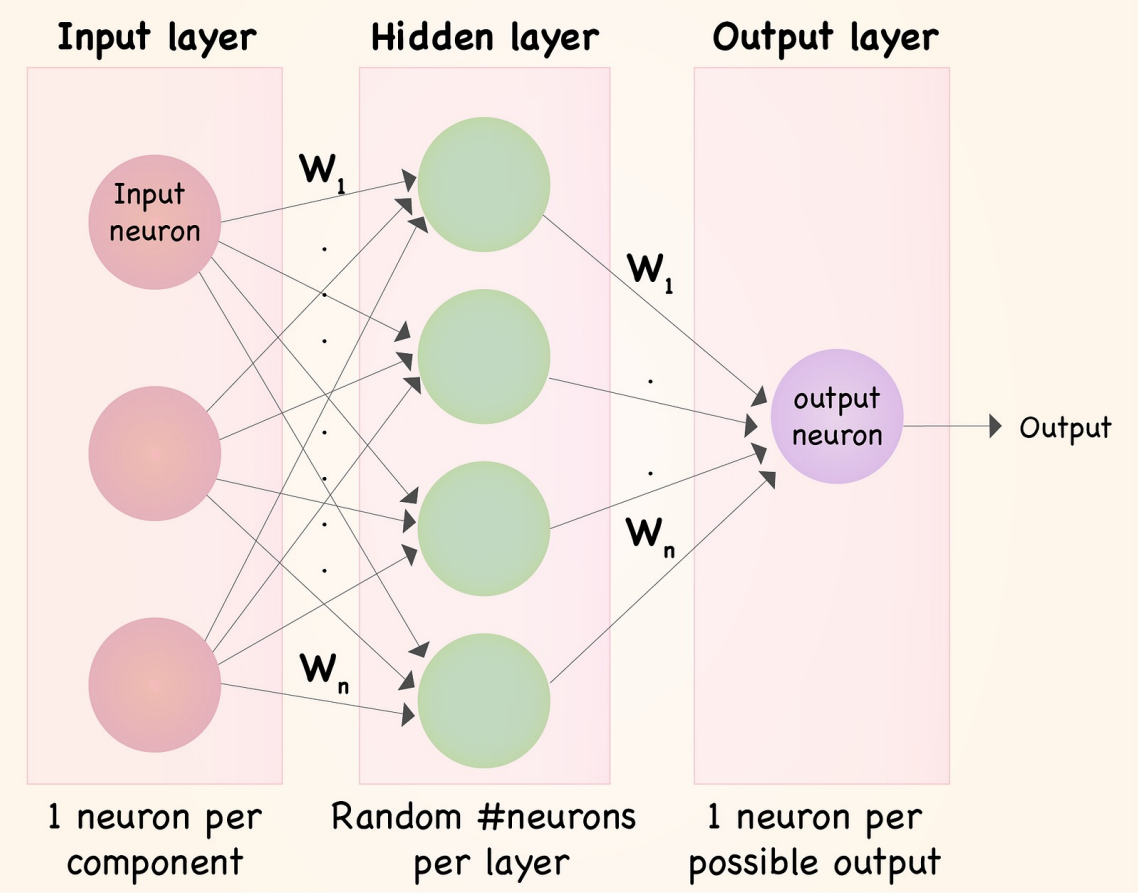




# Deep Learning



## Artificial Neural Network (NN)





Response at scale.

Mid 1800s: The brain is comprised of interconnected neurons.  
**~100 Trillion Connections**

Touching a flame.



Emotions  
Movement



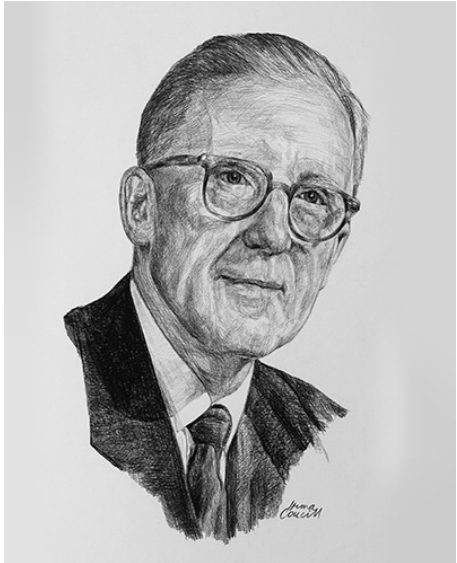
# Connectionism (1873)

- Alexander Bain: philosopher, psychologist, mathematician, logician, linguist, professor
- Main ideas in the book “Mind and Body”
  - Neural groupings
    - Neurons excite and stimulate each other
    - Different input combinations can result in different outputs
    - Activation intensity influences the activation of connected neurons
  - Making memories
    - Neurons connections strengthen with repetitive inputs (Before Hebb’s Law 1949)



# Hebb's Law: Model for Neural Plasticity

- Novelist, schoolteacher, psychologist
- Main idea in book "The Organization of Behavior" (1949):
  - If neuron A repeatedly triggers neuron B, the synapses connecting these neurons get larger.
  - Hebb's Law: "Neurons that fire together wire together."



Response of a neuron  $x_j$

$$x_j = f \left( \sum_{i=1}^N w_i x_i \right)$$

Weights can be different now.

Evolution of synaptic weight

$$\Delta w_{ij} = \eta x_i x_j$$

Weight Update

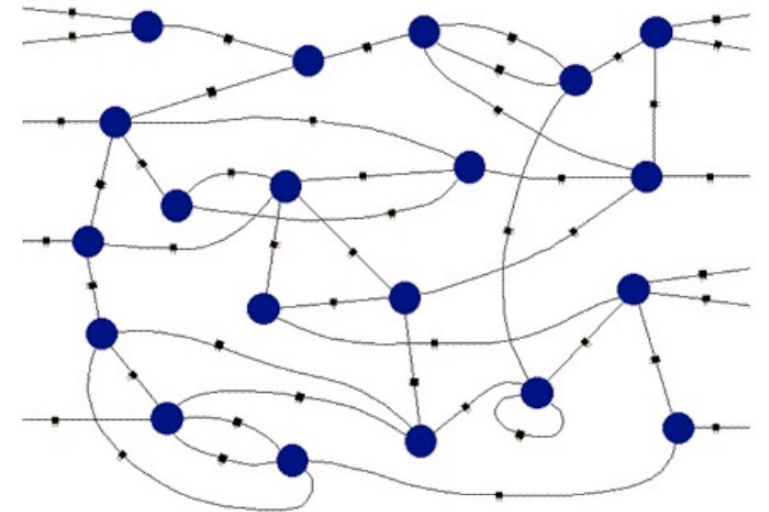
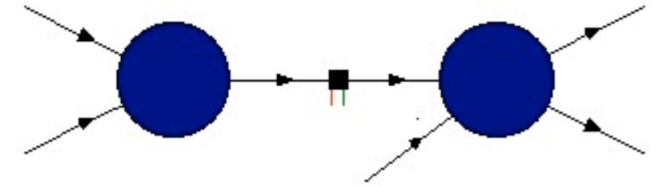
Learning Rate

Interaction between neurons i and j



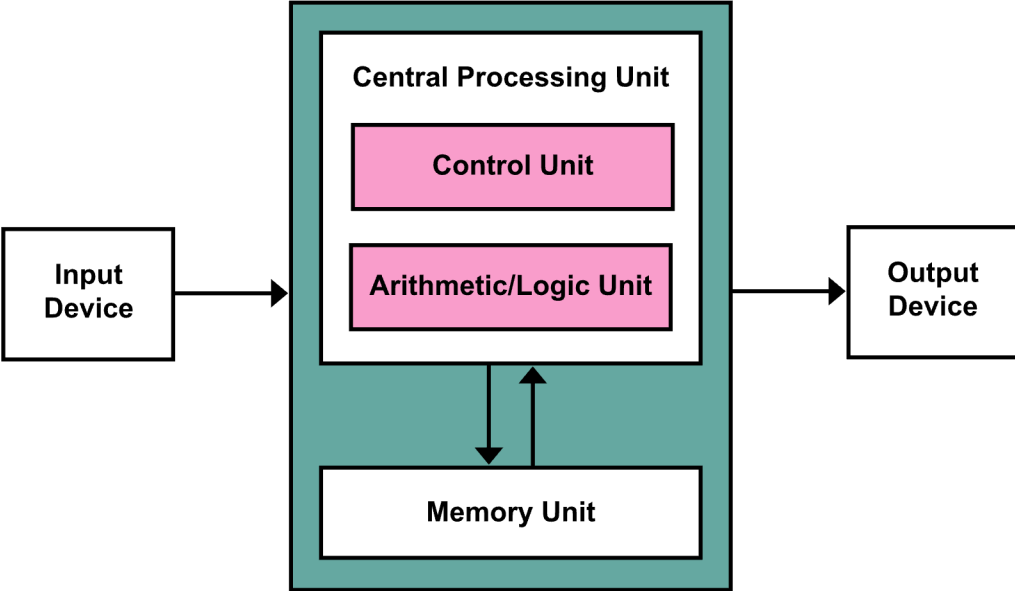
# Connectionist Machines

- Multiple connectionist paradigms proposed
  - Alan Turing's Connectionist model (1948):
  - Parallel Distributed Processing (1986)
    - Rumelhart, Hinton, McClelland
  - Requirements of a connectionist system
    - Bechtel and Abrahamson (1991)
- Main properties
  - Network of processing elements
  - All world knowledge is stored in the connections between the elements



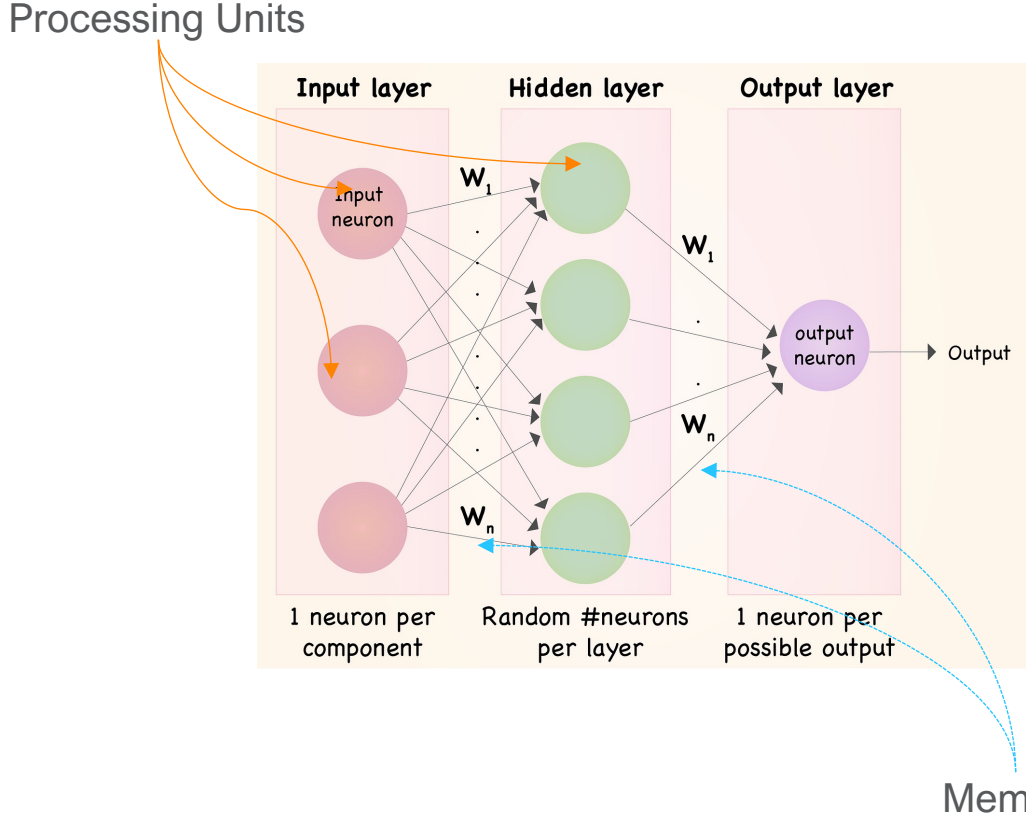
# Von Neumann vs Connectionist Machines

Von Neumann Machines



*The typical modern computer!*

Connectionist Machines





# Pop Quiz

A neural network is a **Von Neumann Machine** because it is a network of processing elements, and all world knowledge is stored in the connections between the elements.

A. True

B. False

# Review

- Hierarchical Clustering
  - There is no need to know the number of clusters beforehand
  - Find inner cluster patterns
  - Explains the relationship between samples
- ANN
  - Connectionism machines
    - Network of processing units
    - Memory is in the connections
  - Key developments
    - Backpropagation
    - ReLU simple activation function
    - Deep Convolutional Networks



# Next Lecture

- Deep Neural Networks



# Helper Slides

