

# Deep Unsupervised Learning (Overview)

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- ▶ We have a dataset without labels. Our goal is to learn something interesting about the underlying structure of the data:
  - Clusters hidden in the dataset.
  - Outliers: particularly unusual and/or interesting data points.
  - Useful signals hidden in the noise, e.g., human speech over a noisy background.

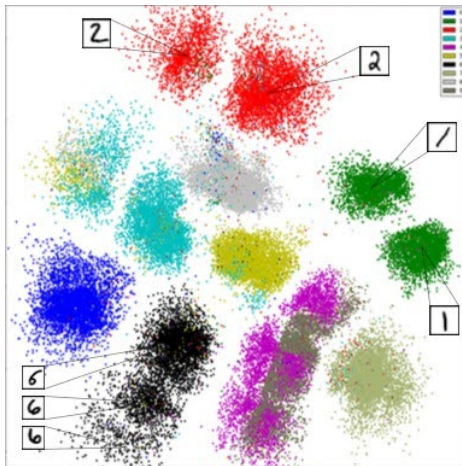
- ▶ **Data:** Unlabeled data, e.g., images, text, or sensor readings.
- ▶ **Model:** A mathematical representation of the data, e.g., a mixture model or a neural network.
- ▶ **Objective function:** A measure of how well the model fits the data, e.g., likelihood or reconstruction error.
- ▶ **Optimization algorithm:** An algorithm to minimize the objective function, e.g., gradient descent or expectation-maximization.
- ▶ **Evaluation metrics:** Measures to assess the quality of the learned model, e.g., silhouette score or clustering accuracy.
- ▶ **Applications:** Use cases for unsupervised learning, e.g., clustering, dimensionality reduction, or anomaly detection.

| Aspect          | Supervised Learning  | Unsupervised Learning  |
|-----------------|--|--|
| Objective       | Learn a function $f$ from labeled input-output pairs.              | Discover structure or representations in unlabeled data.                                 |
| Evaluation      | Accuracy, precision/recall on held-out labels.                     | Clustering validity indices (e.g. silhouette), reconstruction error.                     |
| Cost            | Methods range from $\mathcal{O}(n)$ to $\mathcal{O}(n^3)$ per fit. | k-means $\mathcal{O}(nkd)$ , hierarchical $\mathcal{O}(n^2)$ , PCA $\mathcal{O}(nd^2)$ . |
| Labels/Clusters | Fixed, known set of classes.                                       | Number of clusters unknown; must be chosen or inferred.                                  |
| Output          | Classifier or regressor for new inputs.                            | Cluster assignments, embeddings, density models, or generative samples.                  |

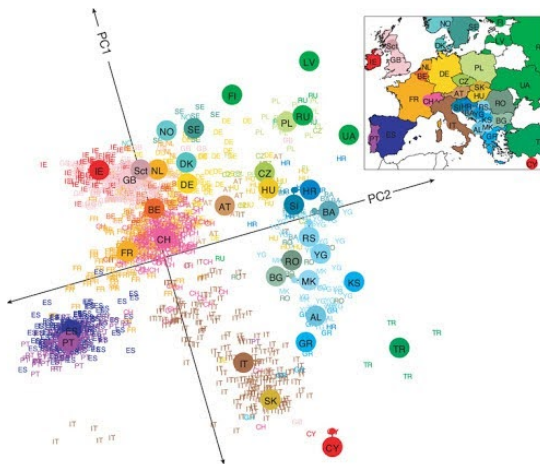
Table 1: Key differences between Supervised and Unsupervised Learning

Unsupervised learning is used in various fields and applications, including:

- ▶ **Visualisation:** Identifying and making accessible useful hidden structures in the data.
- ▶ **Anomaly Detection:** Identifying faulty components that are likely to break soon.
- ▶ **Signal denoising:** Extracting human speech from a noisy recording.
- ▶ **Generative Models:** Learning to generate new data points similar to the training data.
- ▶ **Feature Learning:** Automatically discovering useful representations of the data.
- ▶ **Data Preprocessing:** Cleaning and transforming data for better performance in supervised learning tasks.



**Figure 2:** Unsupervised learning can discover structure in digits without any labels.



**Figure 3:** Dimensionality reduction applied to DNA reveal the geography of European countries.



# What is Deep Unsupervised Learning?

# What is Deep Unsupervised Learning? (cont.)

- ▶ Capturing rich patterns in raw data with deep networks in a label-free way.

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  - **Generative Models:** Recreate raw data distribution.

Why is unsupervised learning challenging?

- ▶ **Exploratory data analysis:** Unsupervised learning is often used for exploratory data analysis, where the goal is to discover patterns or structures in the data without any prior knowledge of the labels.
- ▶ **Difficult to assess performance:** Evaluating the performance of unsupervised learning algorithms can be challenging, as there are no ground truth labels to compare against ("right answer" unknown).
- ▶ **Sensitivity to noise:** Unsupervised learning algorithms can be sensitive to noise and outliers in the data, which can lead to misleading results.
- ▶ **Curse of dimensionality:** As the number of features increases, the data becomes sparse, making it difficult to find meaningful patterns.

## ► Cluster Analysis:

- For identifying homogenous subgroups of samples.
- **Examples:** K-means, hierarchical clustering, DBSCAN.

## ► Dimensionality Reduction:

- For finding a low-dimensional representation to characterize and visualize the data.
- Reducing the number of features in a dataset while preserving important information.
- **Examples:** PCA, t-SNE, UMAP.

## ► Anomaly Detection:

- **Finding outliers in the dataset:** Identifying unusual (rare items, events, or observations) data points that do not conform to expected patterns.
- **Examples:** Isolation Forest, One-Class SVM, Autoencoders.

A set of methods for finding subgroups within the dataset.

- ▶ Observations should share common characteristics within the same group, but differ across groups.
- ▶ Groupings are determined from attributes of the data itself — differs from classification.



Figure 4: Taking a 2 dimensional dataset and separating it into 3 distinct clusters. [Source]

**Input:** Dataset  $D = \{x_1, x_2, \dots, x_n\}$ , number of clusters  $k$

**Output:** Cluster assignments for each data point

**Initialization:** Randomly initialize  $k$  cluster centroids or seeds;

**repeat**

**Assignment Step:** Assign each data point  $x_i$  to the nearest cluster based on a distance metric;

**Update Step:** Recompute cluster centroids using current assignments;

**until** *convergence or maximum iterations reached*;

**return** Final cluster assignments;

**Algorithm:** Generic Clustering Algorithm

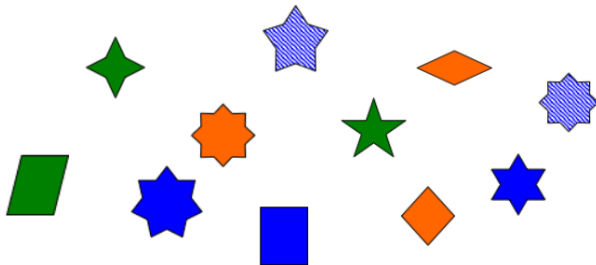


Figure 5: Sample data points.



## Classification

- ▶ Labels available
- ▶ Assigning to known classes
- ▶ Supervised

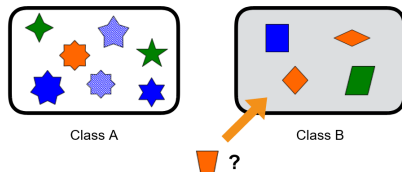


Figure 6: Classification result.

## Clustering

- ▶ No labels
- ▶ Grouping based on similarity
- ▶ Unsupervised

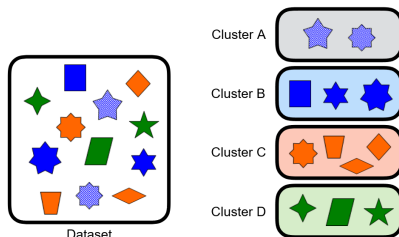


Figure 7: Clustering result.

- ▶ **Centroid-Based Clustering:** Groups data points based on their proximity to a central point, such as K-means or K-medoids.
- ▶ **Hierarchical Clustering:** Builds a hierarchy of clusters using either agglomerative (bottom-up) or divisive (top-down) approaches.
- ▶ **Model-Based Clustering:**
  - Each cluster is represented by a parametric distribution.
  - Dataset is a mixture of distributions.
  - Assumes a probabilistic model for the data and uses statistical methods to identify clusters, such as Gaussian Mixture Models (GMM).
- ▶ **Hard Clustering:**
  - Each data point is assigned exclusively to exactly one cluster.
  - **Example algorithms:** K-means, Hierarchical clustering.

- **interpretation:** No ambiguity — clusters are crisp and non-overlapping.

## ► **Soft/Fuzzy Clustering:**

- Each data point can belong to multiple clusters simultaneously with varying degrees of membership (probabilities or weights).
- **Example algorithms:** Gaussian Mixture Models (GMM), Fuzzy C-means.
- **interpretation:** Reflects uncertainty or mixed membership — clusters can overlap.

Groups data into  $K$  clusters that satisfy two properties.

1. Each observation belongs to at least one of the  $K$  clusters.
2. Clusters are non-overlapping. No observation belongs to more than one cluster.

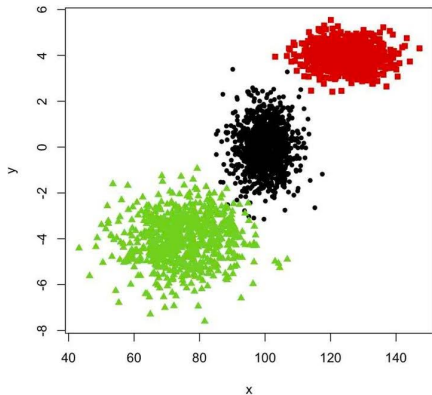


Figure 8: Clusters.

A good clustering is one for which the *within-cluster variation* is as small as possible.

Denote each cluster by  $C_k$ , and let  $W(C_k)$  be a measure of the within-cluster variation.

K-means aims to solve the following optimization problem:

$$\underset{C_1, \dots, C_k}{\text{minimise}} \left\{ \sum_{k=1}^K W(C_k) \right\} \quad (1)$$

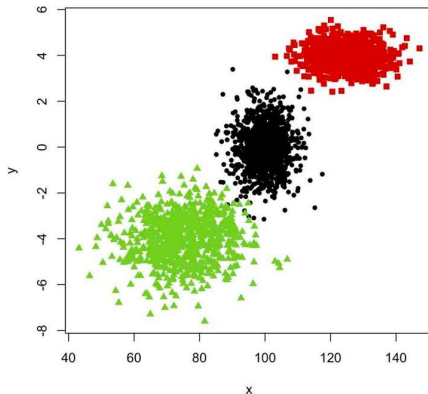


Figure 9: Clusters.

How to measure within-cluster variation?

The most common choice is squared Euclidean distance:

$$W(C_k) = \frac{1}{|C_k|} \sum_{i, i' \in C_k} \sum_{j=1}^p (x_{ij} - x_{i'j})^2 \quad (2)$$

where  $|C_k|$  is the number of points in cluster  $C_k$  and  $x_{ij}$  is the  $j^{th}$  feature of the  $i^{th}$  point.

Which means overall we solve:

$$\text{minimise}_{C_1, \dots, C_k} \left\{ \sum_{k=1}^K \frac{1}{|C_k|} \sum_{i, i' \in C_k} \sum_{j=1}^p (x_{ij} - x_{i'j})^2 \right\} \quad (3)$$

- ▶ It turns out that this optimization problem is difficult to solve, as it is discrete and there are nearly  $K^n$  ways to split  $n$  samples into  $K$  clusters.
- ▶ In practice, use an iterative algorithm that finds a local minimum to this optimization.

**Input:** Dataset  $D = \{x_1, x_2, \dots, x_n\}$ , number of clusters  $k$

**Output:** Cluster assignments for each data point

**Initialization:** Randomly initialize  $k$  cluster centroids or seeds;

**Repeat until convergence:**

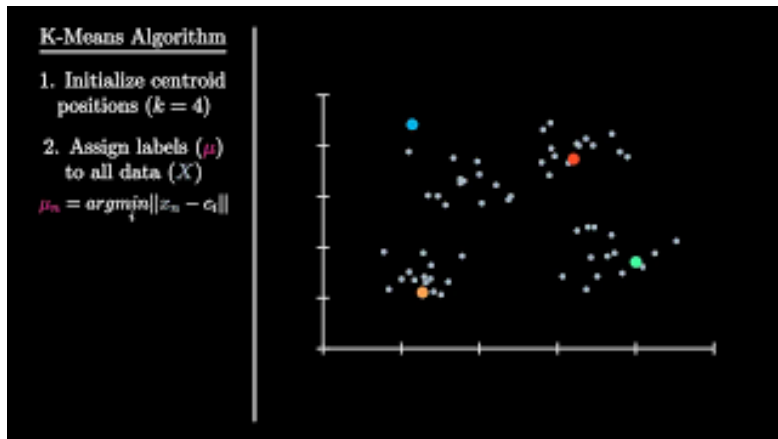
- ▶ **Assignment Step:** Assign each data point  $x_i$  to the nearest cluster based on a distance metric;
- ▶ **Update Step:** Recompute cluster centroids using current assignments;
- ▶ **Convergence Check:** Check if cluster assignments have changed or if centroids have stabilized;

**Return:** Final cluster assignments and centroids;

**Algorithm:** K-means Clustering Algorithm



Watch the K-means clustering algorithm in action:



1. It can be shown that the value of the objective function will never increase at each iteration of  $k$ -means.
2. Since the algorithm finds local minima, however, it will result in different clusters with different initializations.

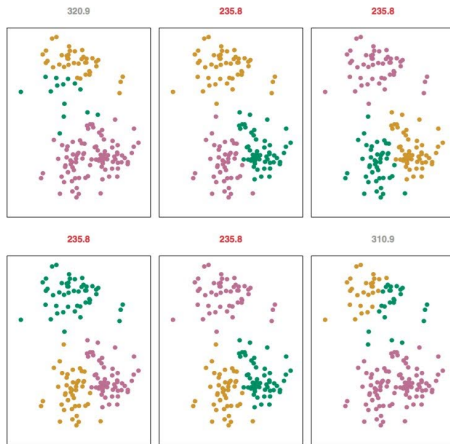


Figure 10: Different initializations of K-means.

## Pros

- ▶ Simple and easy to implement
- ▶ Efficient for large datasets
- ▶ Works well with spherical clusters
- ▶ Scalable to large datasets

## Cons

- ▶ Not robust to data perturbations and different initializations
- ▶ Sensitive to initial centroid placement
- ▶ Assumes spherical clusters
- ▶ Requires specifying the number ' $K$ ' of clusters in advance
- ▶ Sensitive to outliers
- ▶ May converge to local minima
- ▶ Not suitable for non-convex shapes

Cluster based on distances between observations.

Represented as a tree hierarchy (*dendrogram*) rather than a partition of data.

Does not require committing to a choice of  $K$ .

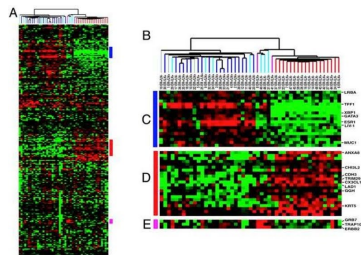


Figure 11: Sørli, Therese, et al. (2003) "Repeated observation of breast tumor subtypes in independent gene expression data sets," PNAS.

- ▶ Each leaf in a dendrogram is a sample/ observation.
- ▶ As we move up the dendrogram, observations that are similar to each other begin to fuse into branches.
- ▶ Branches then fuse into bigger branches.
- ▶ Observations that fuse later (near the top of the tree, or root) are more different than observations that fuse earlier (near the leaves).

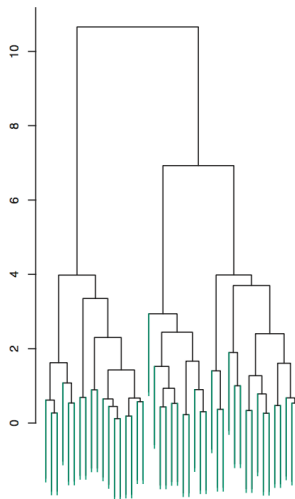


Figure 12: ISL (8th printing 2017)

Note that the horizontal distance between observations on a dendrogram is not the appropriate assessment of observation similarity. Instead, look at vertical axis where branches are first fused.

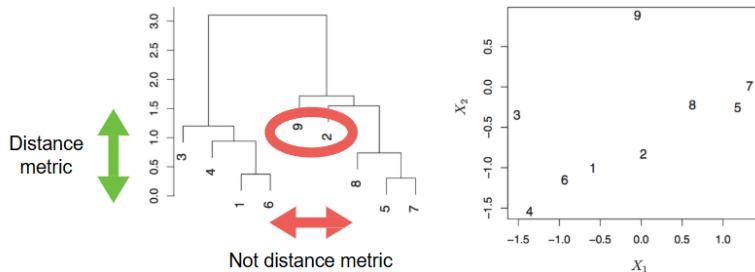


Figure 13: ISL (8th printing 2017)

Clusters are created by making a horizontal cut across the dendrogram. Clusters are the separate trees below the cut.

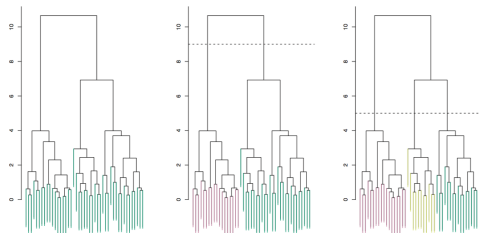


Figure 14: ISL (8th printing 2017)

## Building a Dendrogram

A dendrogram is most commonly built using a bottom-up or agglomerative algorithm.

We start at the leaves and group observations until we reach the root containing the entire dataset.

Like in  $k$ -means, we need a measure of similarity. Again, the most common is Euclidean distance.

- ▶ Compute the distance between each pair of observations.
- ▶ Merge the two closest observations into a cluster.
- ▶ Compute the distance between the new cluster and all other observations.
- ▶ Repeat until all observations are in one cluster.
- ▶ The distance between clusters is computed using a linkage method.



**Input:** Dataset  $D = \{x_1, x_2, \dots, x_n\}$

**Output:** Dendrogram representing the hierarchical structure of clusters

**Initialization:** Treat each data point as a separate cluster;

**Compute distance matrix:** Calculate pairwise distances between all clusters;

**Repeat until only one cluster remains:**

- ▶ Find the two closest clusters based on the distance matrix;
- ▶ Merge the two clusters into a new cluster;
- ▶ Update the distance matrix to reflect the new cluster;
- ▶ Recompute distances between the new cluster and all other clusters using a linkage method;

**Return:** Dendrogram representing the hierarchical structure of clusters;

**Algorithm:** Hierarchical Clustering Algorithm

w3schools: [Codes and Playground](#)

# Clustering - Hierarchical: Dendrograms (cont.)

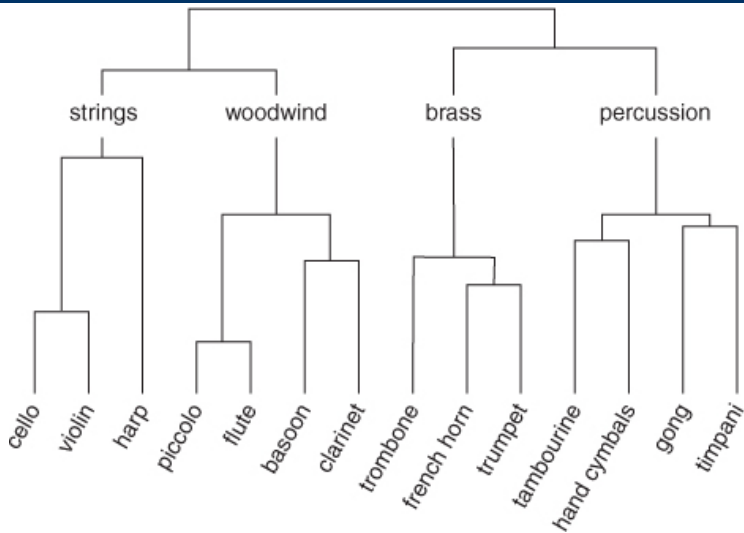


Figure 15: Dendrogram interpretation.

## Distance between groups

It's easy to compute Euclidean distance between two observations. What is the distance or similarity between two groups or clusters of observations?

**Linkage:** defines the dissimilarity between two groups of observations. Most common types are *complete*, *average*, *single*, and *centroid*.

- ▶ **Single Linkage:** Distance between two clusters is the minimum distance between any two points in the clusters.
- ▶ **Complete Linkage:** Distance between two clusters is the maximum distance between any two points in the clusters.
- ▶ **Average Linkage:** Distance between two clusters is the average distance between all pairs of points in the clusters.
- ▶ **Centroid Linkage:** Distance between two clusters is the distance between their centroids.
- ▶ **Ward's Linkage:** Distance between two clusters is the increase in variance when the two clusters are merged.

# Clustering - Hierarchical: Distance Metrics (cont.)

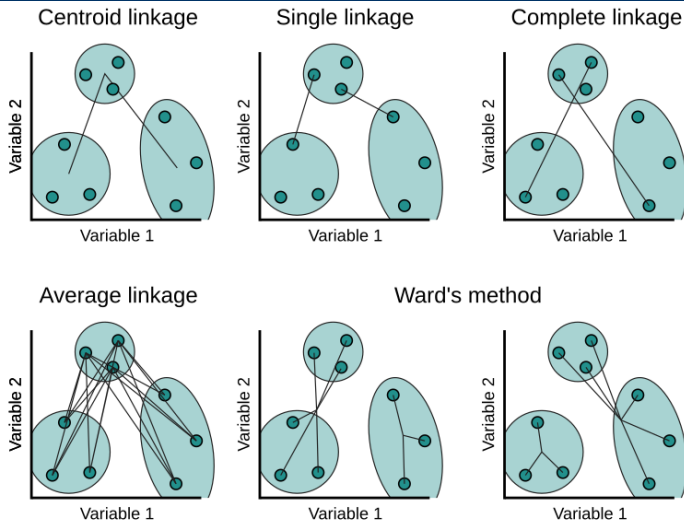


Figure 16: Linkage methods.

# Clustering - Hierarchical: Distance Metrics (cont.)

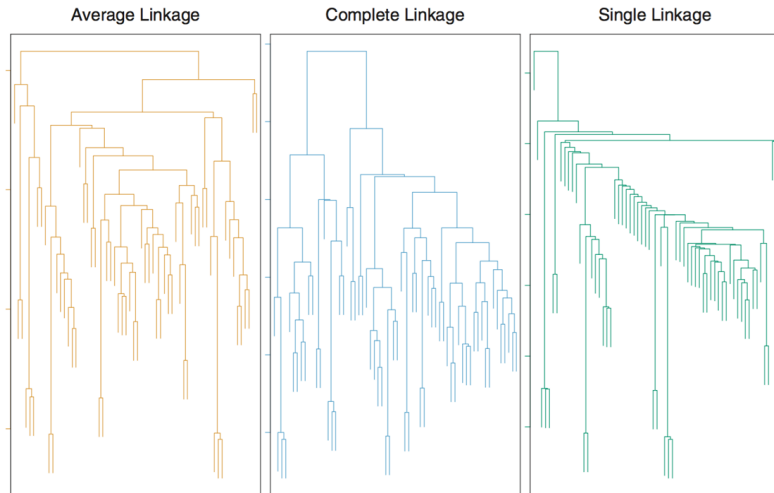


Figure 17: Dendrogram with different linkage types.

## Pros

- ▶ No need to specify the number of clusters  $K$  in advance.
- ▶ Dendrograms provide a visual representation of the clustering process.
- ▶ Can capture complex cluster shapes and relationships.

## Cons

- ▶ Computationally expensive for large datasets.
- ▶ Do have to pick where to cut the dendrogram to obtain clusters
- ▶ Sensitive to similarity measure and type of linkage used.
- ▶ Sensitive to noise and outliers.
- ▶ Difficult to interpret and choose the optimal number of clusters.

## Credits

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