Deep Unsupervised Learning (Overview)

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Unsupervised Learning - Definition

- We have a dataset without labels. Out 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.

Components of Unsupervised Learning

- **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.

Supervised vs Unsupervised Learning

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 - Applications

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

- **Visualisation**: Identifying and making accessiblge useful hidden structures in the data.
- **Anomaly Detection**: Identifying factory 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.

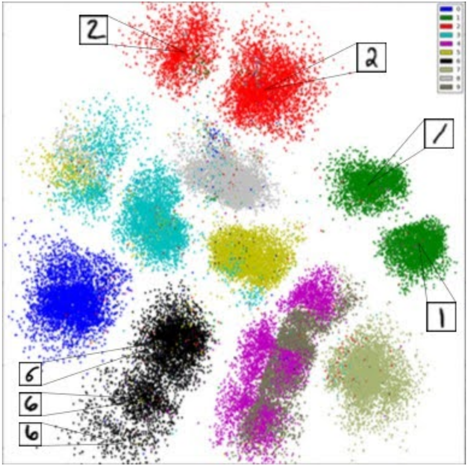


Figure 2: Unsupervised learning can discover structure in digits without any labels.

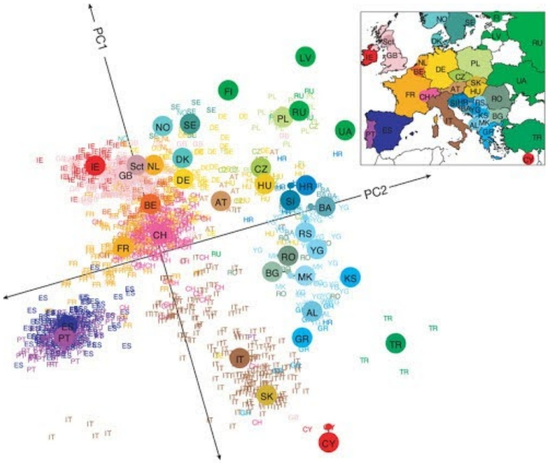


Figure 3: Dimensionality reduction applied to DNA reveal the geography of European countries.

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.

What is Deep Unsupervised Learning? (cont.)

- Capturing rich patterns in raw data with deep networks in a label-free way.
  - **Generative Models**: Recreate raw data distribution.

Unsupervised Learning - Challenges

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.

Unsupervised Learning - Types

- **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.

Clustering

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.

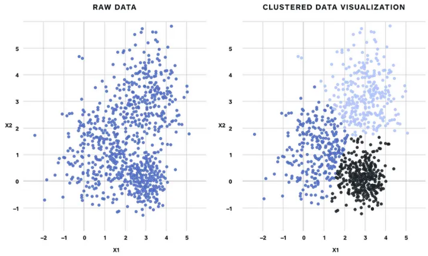


Figure 4: Taking a 2 dimensional dataset and separating it into 3 distinct clusters. [Source]

Clustering (cont.)

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

Clustering Vs Classification

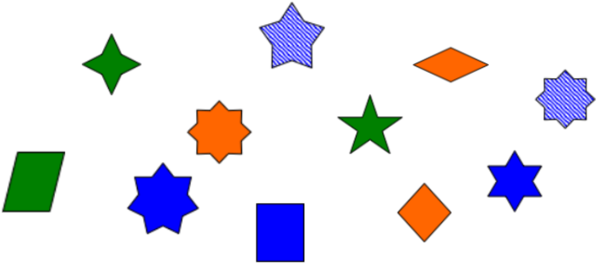


Figure 5: Sample data points.

Clustering Vs Classification (cont.)

Classification
- Labels available
- Assigning to known classes
- Supervised

Clustering
- No labels
- Grouping based on similarity
- Unsupervised

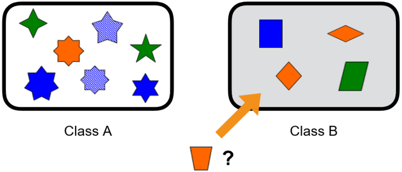


Figure 6: Classification result.

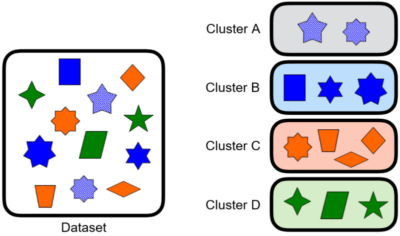


Figure 7: Clustering result.

Clustering: Types

- **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.

Clustering: Types (cont.)

- **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.

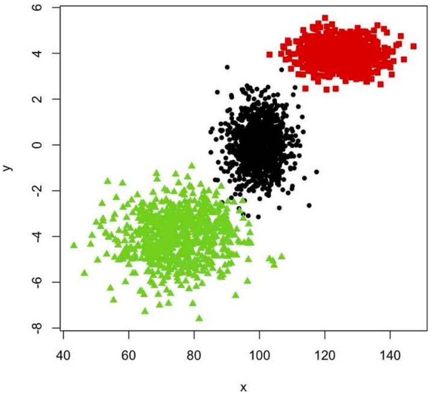


Figure 8: Clusters.

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:

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

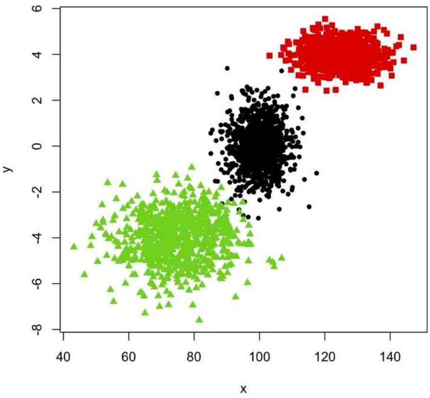


Figure 9: Clusters.

Clustering - K-means (cont.)

How to measure within-cluster variation?

The most common choice is squared Euclidean distance:

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

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:

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

Clustering - K-means (cont.)

- 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 $D = \{x_1, x_2, \ldots, x_n\}$, number of clusters k
Output: Cluster assignments for each data point

Initialization: Randomly initialize k cluster centroids or seeds;

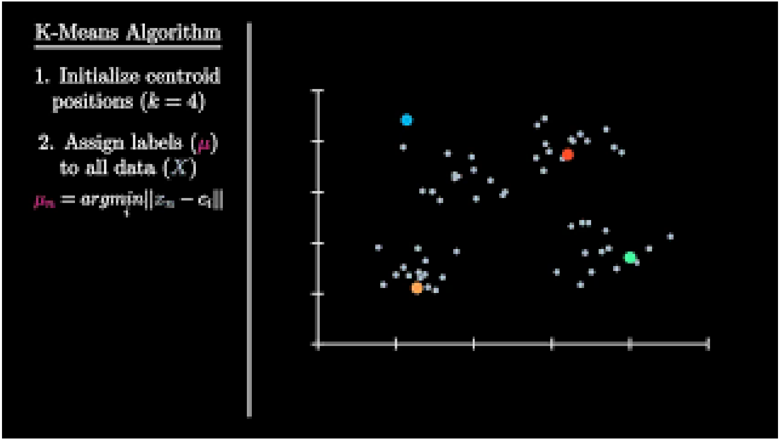
Repeat until convergence:

- **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.

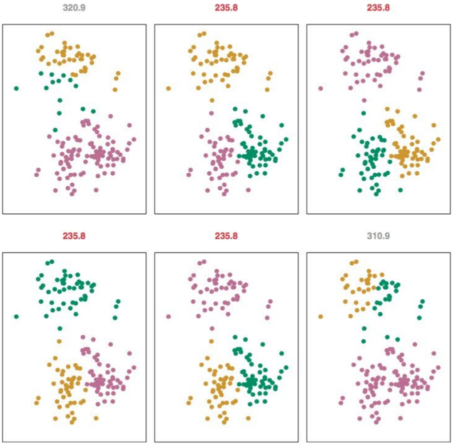


Figure 10: Different initializations of K-means.

K-means - Pros and Cons

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.

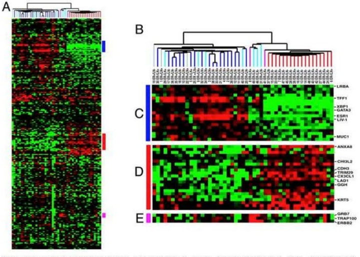


Figure 11: Sørlie, Therese, et al. (2003) "Repeated observation of breast tumor subtypes in independent gene expression data sets," PNAS.

- 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).

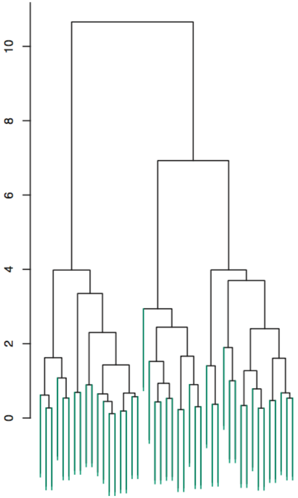


Figure 12: ISL (8th printing 2017)

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.

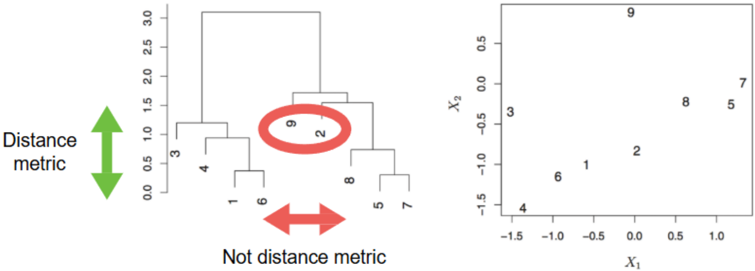


Figure 13: ISL (8th printing 2017)

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

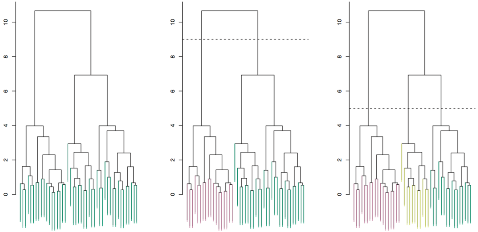


Figure 14: ISL (8th printing 2017)

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 $D = \{x_1, x_2, \ldots, x_n\}$
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.)

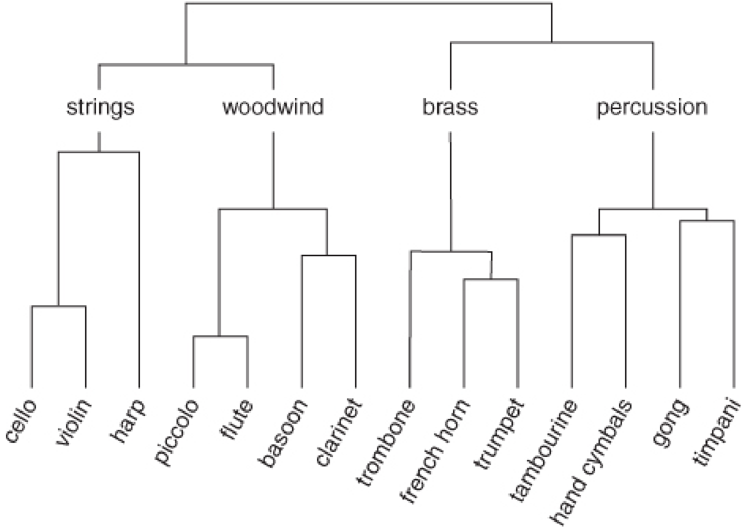


Figure 15: Dendrogram interpretation.

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*.

Clustering - Hierarchical: Distance Metrics (cont.)

- **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.

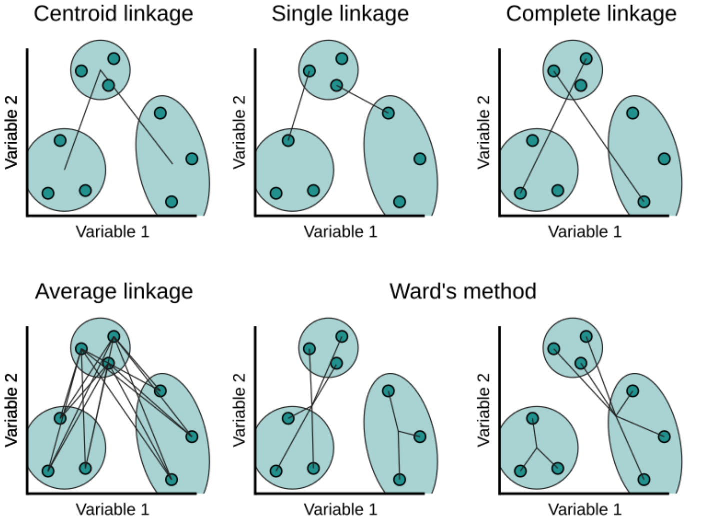


Figure 16: Linkage methods.

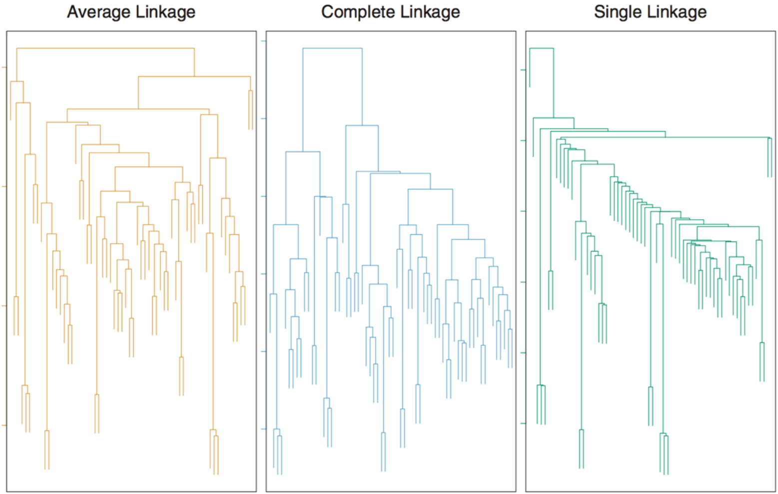


Figure 17: Dendrogram with different linkage types.

Clustering - Hierarchical: Pros and Cons

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.

Clustering - Density-Based Methods

- Clustering based on density (local cluster criterion), such as density-connected points or based on an explicitly constructed density function.
- **Major features**:
  - Discover clusters of arbitrary shape
  - Handle noise
  - One scan
  - Need density parameters

- **Major algorithms**:
  - DBSCAN (Density-Based Spatial Clustering of Applications with Noise): Ester, et al. (KDD'96)
  - OPTICS (Ordering Points to Identify the Clustering Structure): Ankerst, et al. (SIGMOD'99)
  - HDBSCAN (Hierarchical Density-Based Spatial Clustering of Applications with Noise): Campello, et al. (ACM TIST'15)
  - DENCLUE (DENsity-based CLUstEring): Hinneburg and Gabriel (KDD'97)
  - CLIQUE (CLustering In QUEst): Karypis, Han, and Kumar (SIGMOD'98)

- **DBSCAN** (Density-Based Spatial Clustering of Applications with Noise):
  - Density = number of points within a specified radius ϵ.
  - A point is a core point if it has more than a specified number of points (MinPts) within ϵ. These are points that are at the interior of a cluster.
  - A border point has fewer than MinPts within ϵ, but is in the neighborhood of a core point
  - A noise point is any point that is not a core point or a border point.
  - Groups together points that are closely packed together, marking as outliers points that lie alone in low-density regions.
  - Parameters:
    - ϵ: Maximum distance between two points for them to be considered as in the same neighborhood.
    - MinPts: Minimum number of points required to form a dense region.

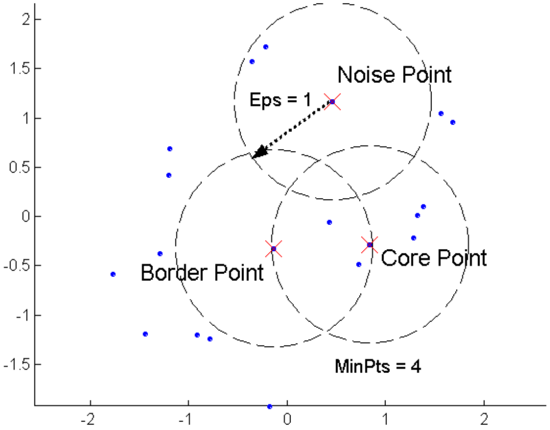


Figure 18: DBSCAN features: Core, Border, and Noise Points

Input: Set of points P, distance threshold ε, minimum number of points *minPts*

Output: A set of clusters

Construct a directed graph $G = (V, E)$ where each node in V corresponds to a point in P;

foreach *point* $c \in P$ **do**

  if *c is a core point (i.e., $|\mathcal{N}_\varepsilon(c)| \geq minPts$)* **then**

    foreach *point* $p \in \mathcal{N}_\varepsilon(c)$ **do**

      Add a directed edge $(c \to p)$ to E;

    end

  end

end

$N \leftarrow V$;

while *there exists a core point* $c \in N$ **do**

  Let X be the set of nodes reachable from c via directed edges in G;

  Form a cluster $C = X \cup \{c\}$;

  Remove all nodes in C from N;

end

Algorithm: Graph-Based DBSCAN Clustering

Credits

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