Clustering Analysis

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Overview

Clustering

- Clustering is an interesting problem of **unsupervised learning** $\rightarrow$ cluster analysis does not use category labels that tag objects with prior identifiers.
- Deals with **data structure partitioning** in space.
- Forms the basis of **exploratory data analysis (EDA).**
- The idea of clusters is intuitively accessible.

A cluster is comprised of a number of *similar* objects.

- It is interesting to see how one might go about formally defining clusters.

Defining Clusters

- A cluster is a set of entities which are **alike**, and entities from different clusters are not.
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Everitt, B. S. (1974). *Cluster Analysis*. John Wiley & Sons, Inc., New York.

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- Clusters may be described as connected regions of a multidimensional space containing a relatively **high density** of points separated from other such regions by a region containing a relatively low density of points.

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The last two definitions assume that objects to be clustered are represented as points in measurement space, and that this is the premise from now on.

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Clustering Techniques

- Centroid-Based Techniques
- Density-Based Techniques

Distance Functions

$$\mathbf{X} = (x_1, x_2, x_3, \ldots, x_n), \mathbf{Y} = (y_1, y_2, y_3, \ldots, y_n) \in \mathbb{R}^n$$

City Block Distance

$$\mathcal{D}(\mathbf{X},\mathbf{Y}) = \sum_i^n |x_i - y_i|$$

Euclidean Distance

$$\mathcal{D}(\mathbf{X},\mathbf{Y}) = (\sum_i^n (x_i - y_i)^2)^{\frac{1}{2}}$$

Chebyshev Distance

$$\mathcal{D}(\mathbf{X},\mathbf{Y}) = \mathscr{M}(|x_i - y_i|)$$

Minkowski Distance

$$\mathcal{D}(\mathbf{X},\mathbf{Y}) = (\sum_i^n (x_i - y_i)^p)^{\frac{1}{p}}$$

Minkowski Distance

- $p = 1$ (City Block Distance)
- $p = 2$ (Euclidean Distance)
- $p \to \infty$ (Chebyshev Distance)

Clustering Algorithms

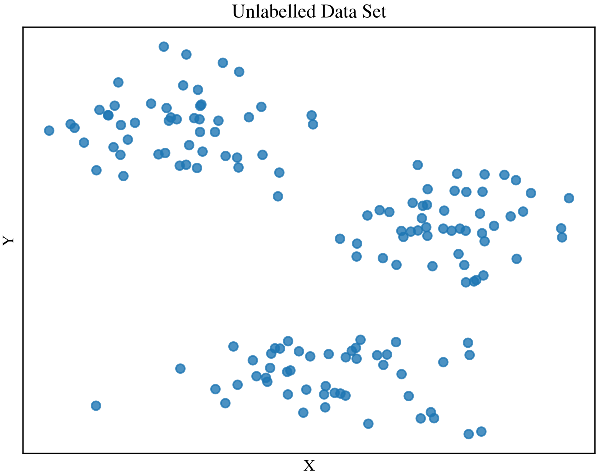
- K-Means Algorithm
- DBSCAN
- HDBSCAN

K-Means Algorithm[1]

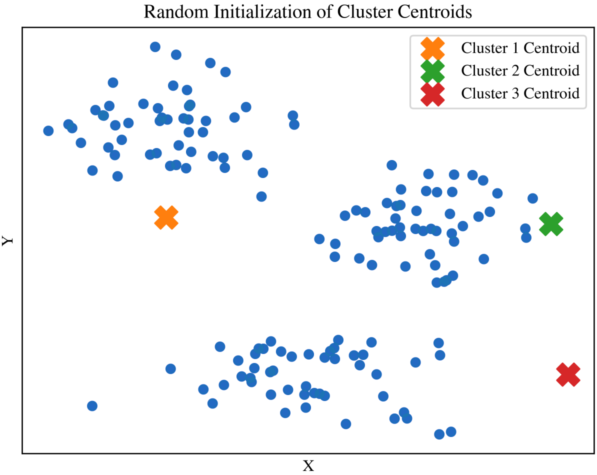
1. Randomly initialize K centroids.
2. Calculate distance of each point ($\mathbf{X}_i$) from each of the K centroids.
3. Assign each point ($\mathbf{X}_i$) to the centroid located at minimum distance.
4. Update the centroids by computing the mean of points assigned to each cluster.
5. Go to 2.

[1] S. Lloyd. "Least squares quantization in PCM". In: *IEEE Transactions on Information Theory* 28.2 (1982), pp. 129–137. DOI: 10.1109/TIT.1982.1056489.

Visualizing the *K*-Means Algorithm



Visualizing the *K*-Means Algorithm



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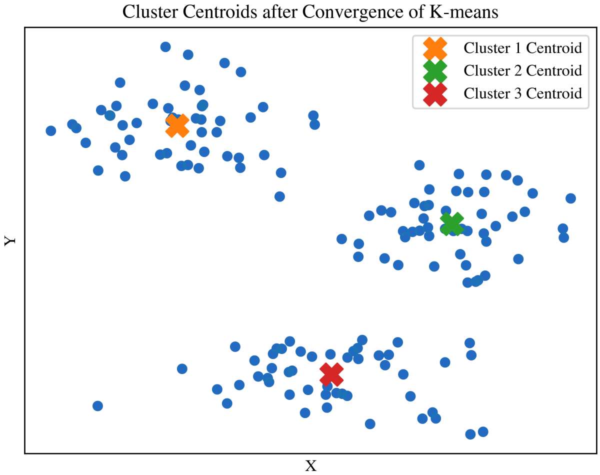

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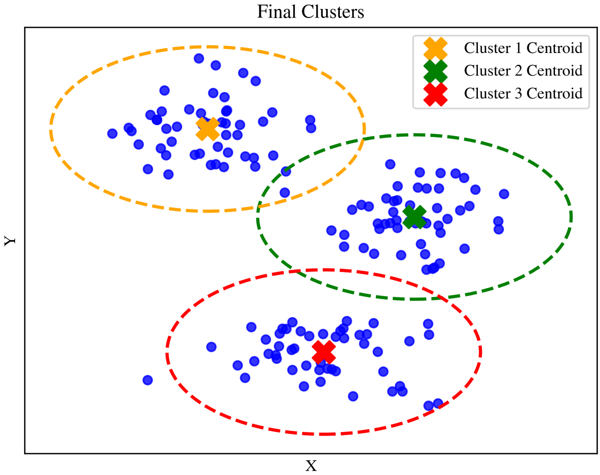

The Fall of K-Means

1. What is K?
2. K-Means is sensitive to initial conditions.
3. K-Means can't handle "nested" clusters.

The Fall of K-Means

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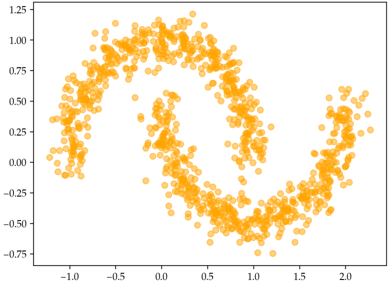

Figure: *Two Moons* Data Set

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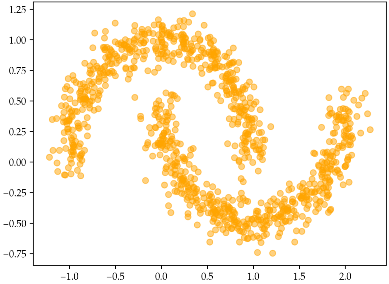

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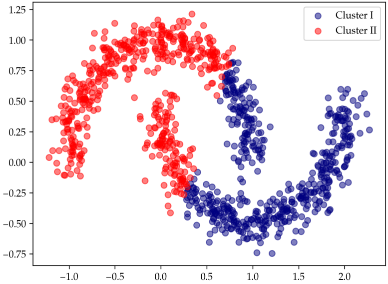

Figure: K-Means on *Two Moons*

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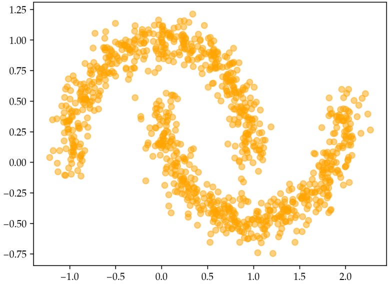

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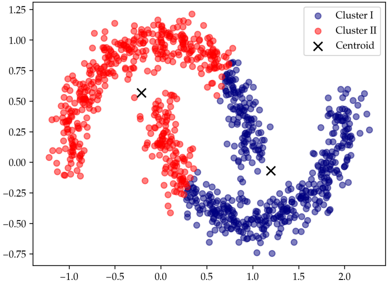

Figure: K-Means on *Two Moons*

DBSCAN[1] (Density-Based Spatial Clustering of Applications with Noise)

Identifying Clusters by Visual Inspection

Clusters are defined by high density regions. **Outliers** are defined by low density regions.

1. For each point in the data, check if there are at least η points around it at ϵ distance from it. Every point that satisfies this criterion is said to be a **Core**. Others are **Non-Cores**.
2. Start with a random core point. Add itself and all the cores around it that are at least ϵ distance from it to one cluster.
3. Let the clusters grow until there are only cores in each cluster. After that, add all non-cores that are at least ϵ distance from any of the cores to the respective clusters. These are **Boundary Points**.
4. The remaining points are labelled as outliers.

[1] Martin Ester et al. "A density-based algorithm for discovering clusters in large spatial databases with noise". In: *Proceedings of the Second International Conference on Knowledge Discovery and Data Mining*. 1996, pp. 226–231.

DBSCAN in Action

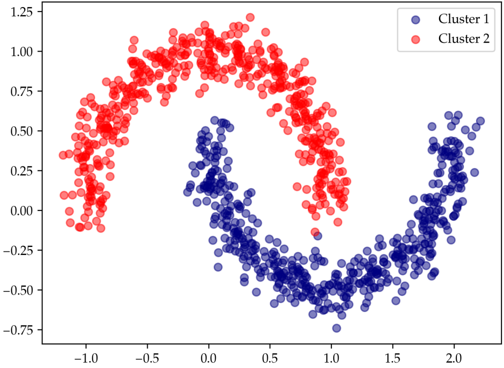

Figure: DBSCAN on *Two Moons* ($\eta = 4$, $\epsilon = 0.1$)

The Fall of DBSCAN

1. What are η & ϵ?
2. Does not do well with real-world data that is affected by noise.

The Fall of DBSCAN

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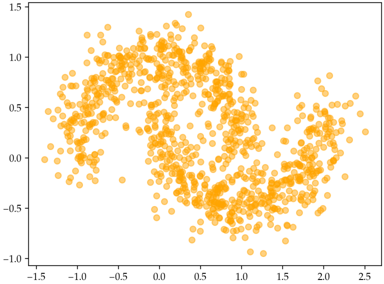

Figure: *Two Moons* Data Set (noise = 0.18)

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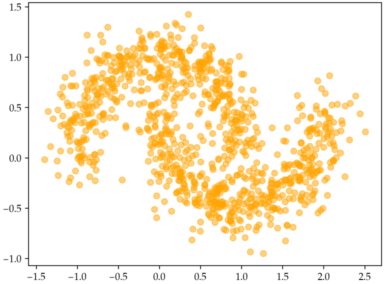

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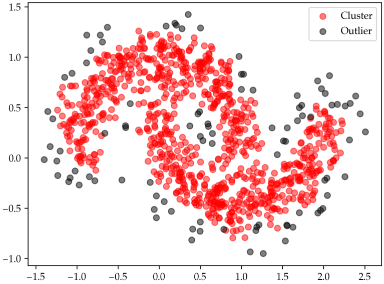

Figure: DBSCAN on noisy *Two Moons*

HDBSCAN[2]

(Hierarchical Density-Based Spatial Clustering of Applications with Noise)

1. Lower the "sea" level using: $\mathrm{d}_k(a, b) = \max\{\mathrm{core}_k(a), \mathrm{core}_k(b), \mathrm{d}_{a,b}\}$[1]. k denotes the k^{th} nearest neighbour.
2. Consider the data as a weighted graph with the data points as vertices and an edge between any two points with weight equal to the d_k of those points.
3. Make a dendrogram, starting with each point as a single cluster and ending with one large cluster of all points.
4. Prune the dendrogram whenever there there are less than m number of points in a cluster.

[1] Justin Eldridge, Mikhail Belkin, and Yusu Wang. "Beyond Hartigan Consistency: Merge Distortion Metric for Hierarchical Clustering". In: *Proceedings of The 28th Conference on Learning Theory*. Vol. 40. Proceedings of Machine Learning Research. Paris, France, Mar. 2015, pp. 588–606.

[2] Leland McInnes, John Healy, and S. Astels. "hdbscan: Hierarchical density based clustering". In: *J. Open Source Softw.* 2 (2017), p. 205.

HDBSCAN in Action

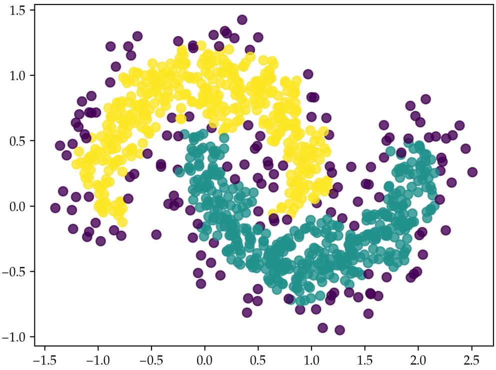

Figure: HDBSCAN on *Two Moons* ($\eta = 4$, $m = 400$)

Summary

- Clustering is an important problem concerning unsupervised learning algorithms.
- Distance metrics are important for discerning similarity or dissimilarity.
- K-Means is a centroid-based algorithm. It requires a judicious choice of K. Further, it makes assumptions about the nature of the shape of clusters $\rightarrow$ the Gaussian "ball" assumption.
- DBSCAN is a density-based algorithm. It performs poorly on data sets containing clusters of varying densities.
- HDBSCAN is a hierarchical density-based algorithm. It improves upon DBSCAN.

References

[1] S. Lloyd. "Least squares quantization in PCM". In: *IEEE Transactions on Information Theory* 28.2 (1982), pp. 129–137. DOI: 10.1109/TIT.1982.1056489.

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