CSC 461: Machine Learning

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Hierarchical Clustering

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Hierarchical clustering

- Unsupervised learning technique that groups observations into nested clusters
- Key features:
  - does not require a predefined number of clusters
  - creates a hierarchy of clusters, often visualized as a dendrogram
    - can be agglomerative (bottom-up), or divisive (top-down)
  - widely used in various domains (gene expression, phylogenetic trees, community detection, etc.)

Agglomerative vs divisive

- Agglomerative approach (**bottom-up**)
  - start with observations as singleton clusters and progressively merge them until a final single cluster is created
  - most common form
- Divisive approach (**top-down**)
  - start with all observations on a single cluster and progressively split the clusters until all observations are singleton clusters

HAC algorithm

- Initially each observation is considered a cluster
- Repeat
  - **merge:** find the closest pair of clusters and merge it into a single cluster
  - if all observations are in a single cluster stop

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Distance Metrics:
 – Euclidean distance
 – Manhattan distance
 – Minkowski distance
 – Hamming distance
 – Cosine similarity
 – Correlation coefficient

Linkage Criteria:
 – Single–linkage
 – Complete–linkage
 – Average–linkage
 – Centroid–linkage
 – Ward's method
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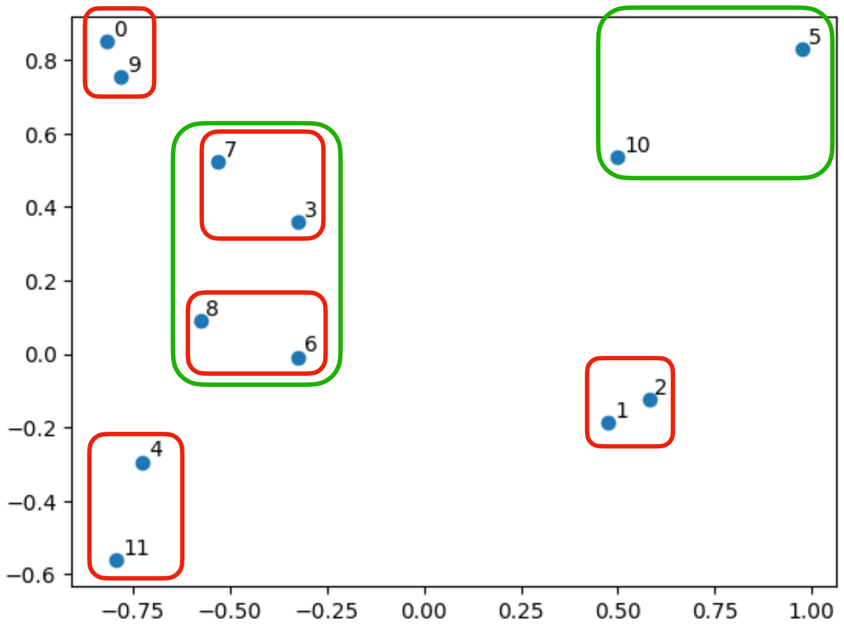
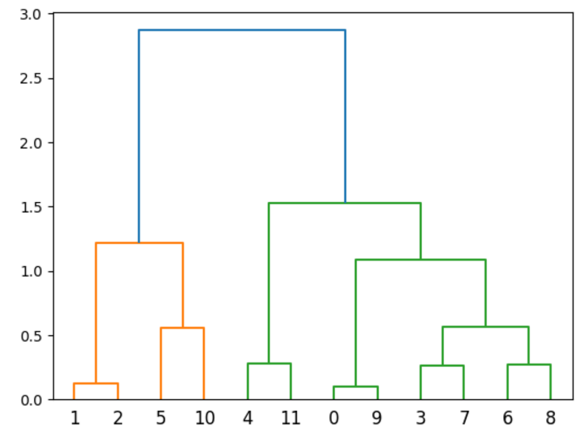


Dendrogram

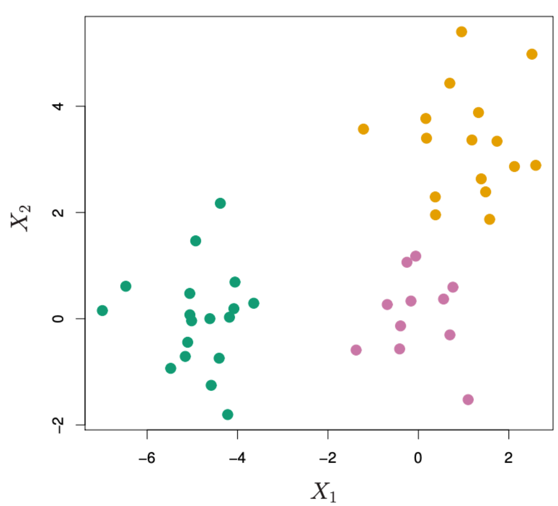


A dendrogram represents the hierarchy of clusters

Y-axis represents the distance at which clusters are merged

Horizontal cuts through the dendrogram represent cluster groupings at various thresholds

Consider this data



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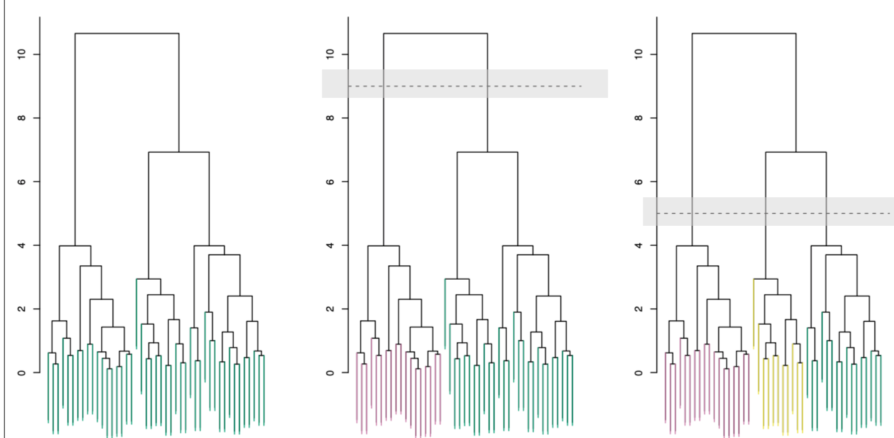
HAC with complete-linkage



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Pairwise metrics

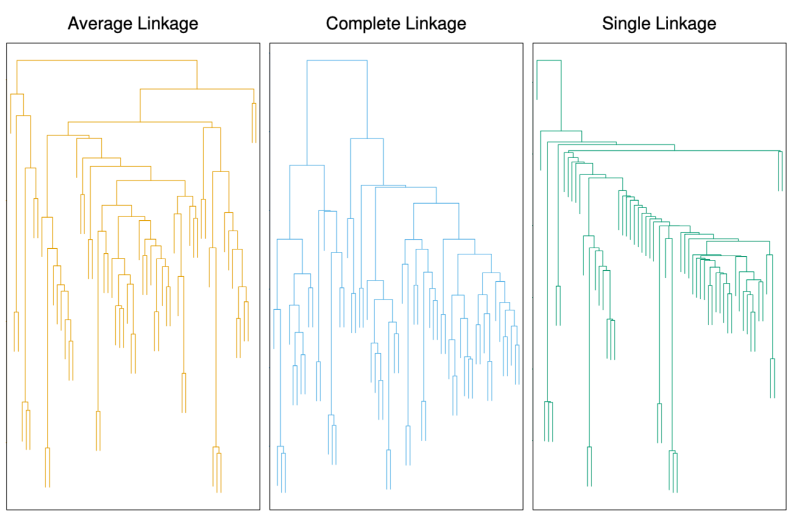
See the Pairwise metrics, Affinities and Kernels section of the user guide for further details.

`metrics.pairwise.additive_chi2_kernel`(X[, Y])	Compute the additive chi-squared kernel between observations in X and Y.
`metrics.pairwise.chi2_kernel`(X[, Y, gamma])	Compute the exponential chi-squared kernel between X and Y.
`metrics.pairwise.cosine_similarity`(X[, Y, ...])	Compute cosine similarity between samples in X and Y.
`metrics.pairwise.cosine_distances`(X[, Y])	Compute cosine distance between samples in X and Y.
`metrics.pairwise.distance_metrics`()	Valid metrics for pairwise_distances.
`metrics.pairwise.euclidean_distances`(X[, Y, ...])	Compute the distance matrix between each pair from a vector array X and Y.
`metrics.pairwise.haversine_distances`(X[, Y])	Compute the Haversine distance between samples in X and Y.
`metrics.pairwise.kernel_metrics`()	Valid metrics for pairwise_kernels.
`metrics.pairwise.laplacian_kernel`(X[, Y, gamma])	Compute the laplacian kernel between X and Y.
`metrics.pairwise.linear_kernel`(X[, Y, ...])	Compute the linear kernel between X and Y.
`metrics.pairwise.manhattan_distances`(X[, Y, ...])	Compute the L1 distances between the vectors in X and Y.
`metrics.pairwise.nan_euclidean_distances`(X)	Calculate the euclidean distances in the presence of missing values.
`metrics.pairwise.pairwise_kernels`(X[, Y, ...])	Compute the kernel between arrays X and optional array Y.
`metrics.pairwise.polynomial_kernel`(X[, Y, ...])	Compute the polynomial kernel between X and Y.
`metrics.pairwise.rbf_kernel`(X[, Y, gamma])	Compute the rbf (gaussian) kernel between X and Y.
`metrics.pairwise.sigmoid_kernel`(X[, Y, ...])	Compute the sigmoid kernel between X and Y.
`metrics.pairwise.paired_euclidean_distances`(X, Y)	Compute the paired euclidean distances between X and Y.
`metrics.pairwise.paired_manhattan_distances`(X, Y)	Compute the paired L1 distances between X and Y.
`metrics.pairwise.paired_cosine_distances`(X, Y)	Compute the paired cosine distances between X and Y.
`metrics.pairwise.paired_distances`(X, Y, *[, ...])	Compute the paired distances between X and Y.
`metrics.pairwise_distances`(X[, Y, metric, ...])	Compute the distance matrix from a vector array X and optional Y.
`metrics.pairwise_distances_argmin`(X, Y, *[, ...])	Compute minimum distances between one point and a set of points.
`metrics.pairwise_distances_argmin_min`(X, Y, *)	Compute minimum distances between one point and a set of points.
`metrics.pairwise_distances_chunked`(X[, Y, ...])	Generate a distance matrix chunk by chunk with optional reduction.

Distances between clusters

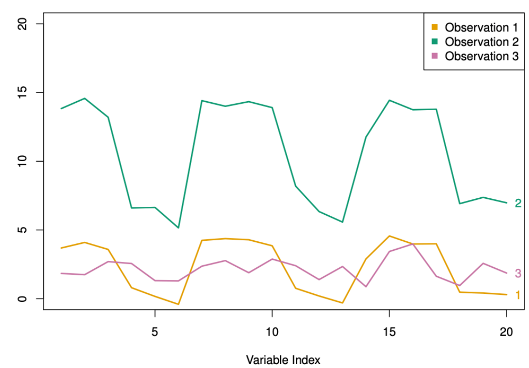
Single-linkage:	$D(A,B) = \underset{\mathbf{x}_1 \in A, \mathbf{x}_2 \in B}{\arg\min}\ d(\mathbf{x}_1, \mathbf{x}_2)$
Complete-linkage:	$D(A,B) = \underset{\mathbf{x}_1 \in A, \mathbf{x}_2 \in B}{\arg\max}\ d(\mathbf{x}_1, \mathbf{x}_2)$
Average-linkage:	$D(A,B) = \frac{1}{\lvert A \rvert \lvert B \rvert} \sum_{\mathbf{x}_1 \in A, \mathbf{x}_2 \in B} d(\mathbf{x}_1, \mathbf{x}_2)$
Centroid-linkage:	$D(A,B) = \lVert \mu_A - \mu_B \rVert_2^2$
Ward's method:	Minimizes variance within clusters

Example



What kind of distance to consider?

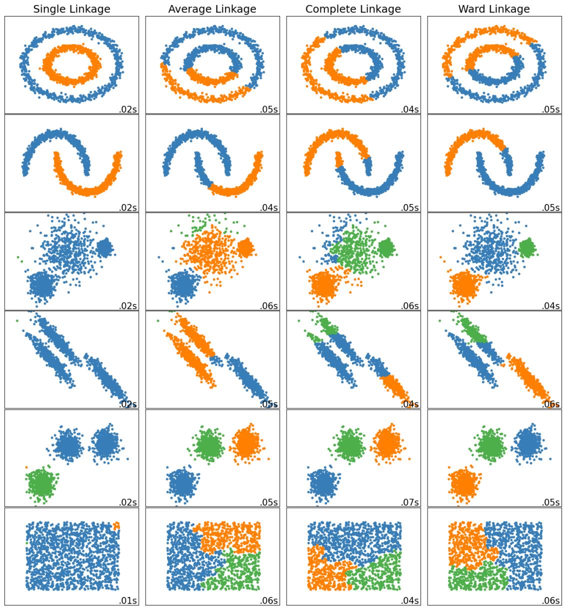
- We have been using Euclidean distances, however, the choice is **very important**



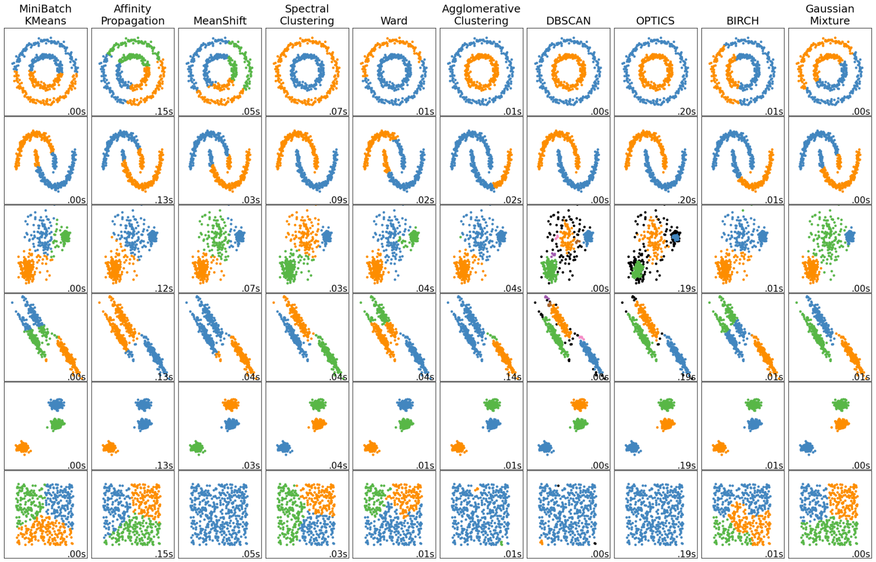
Observations 1 and 3 have a small Euclidean distance between them. But they have a large correlation-based distance. Observations 1 and 2 have a large Euclidean distance between them. But they have a small correlation-based distance.

Limitations and considerations

- Computational complexity
  - can be computationally expensive for large datasets
- Sensitivity to noise and outliers
  - can be sensitive to noise and outliers in the data
- Choice of distance metric and linkage criterion
  - distance metric and linkage criterion can significantly affect the results
- Optimal number of clusters
  - no definitive method for determining the optimal number of clusters



From scikit-learn



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