

Hierarchical Clustering 101

Hierarchical Clustering

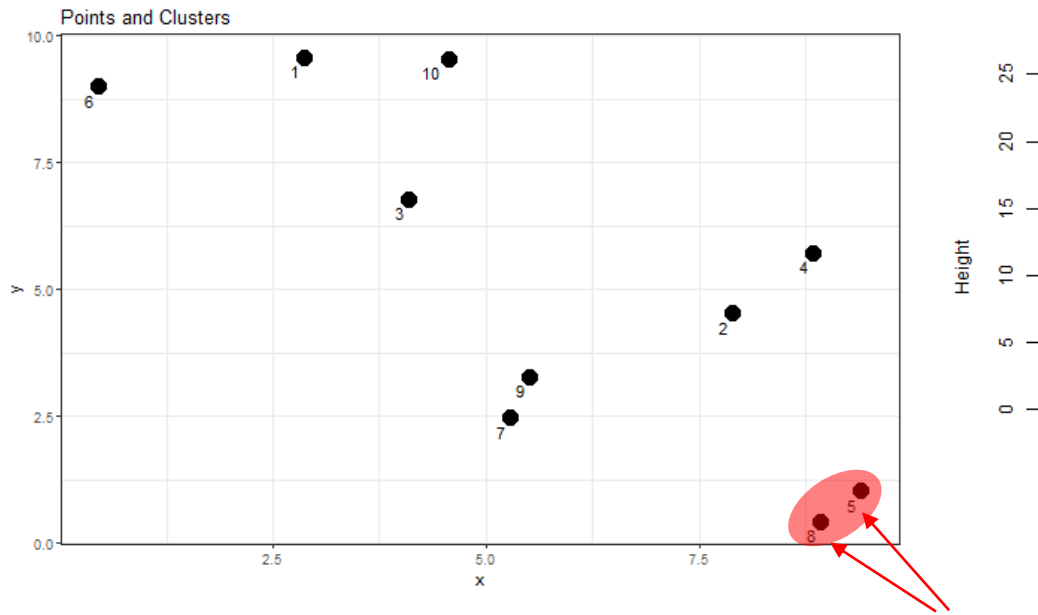
Introduction

- Algorithm for building **clusters** based on **hierarchy**
- Assesses similarity (distance) of observations
- Result is visualised as dendrogram
- Bottom-up approach
 - each point individual cluster
 - gradually join points
 - Start with most similar points
- Top-down approach
 - All points in one cluster
 - Split clusters until desired cluster number reached
- Depends on two important parameters
 - Distance metric
 - Linkage

Hierarchical Clustering

How the dendrogram is created

- Find closest pair of points



closest pair of points: 5 and 8

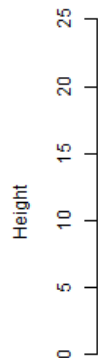
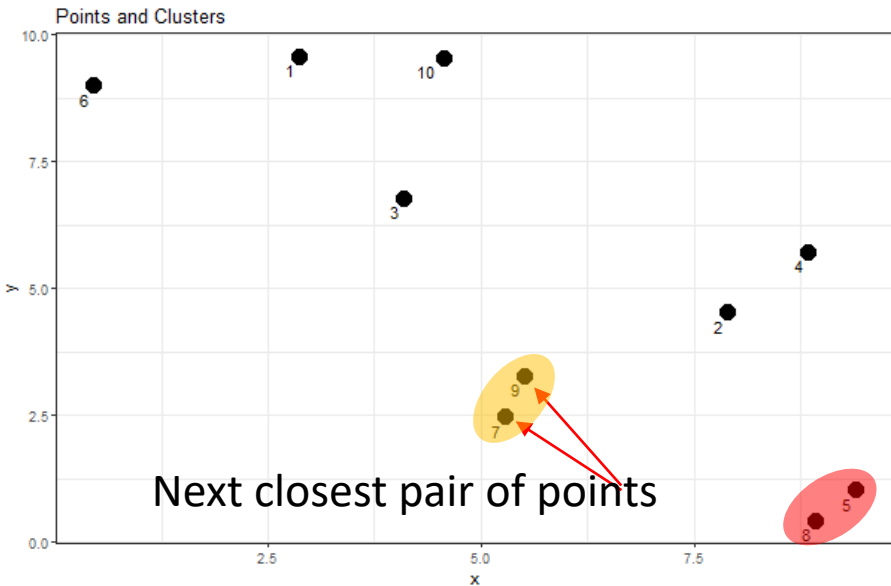
Height represents distance

```
distance_mat  
hclust(*, "ward.D")
```

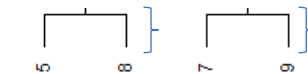
Hierarchical Clustering

How the dendrogram is created

- Then find next closest pair of points



Similar height →
Similar distance

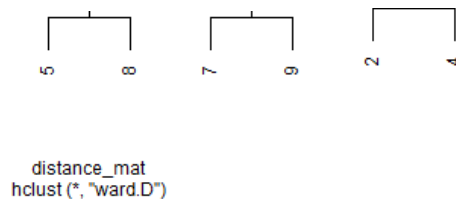
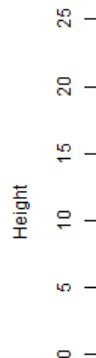
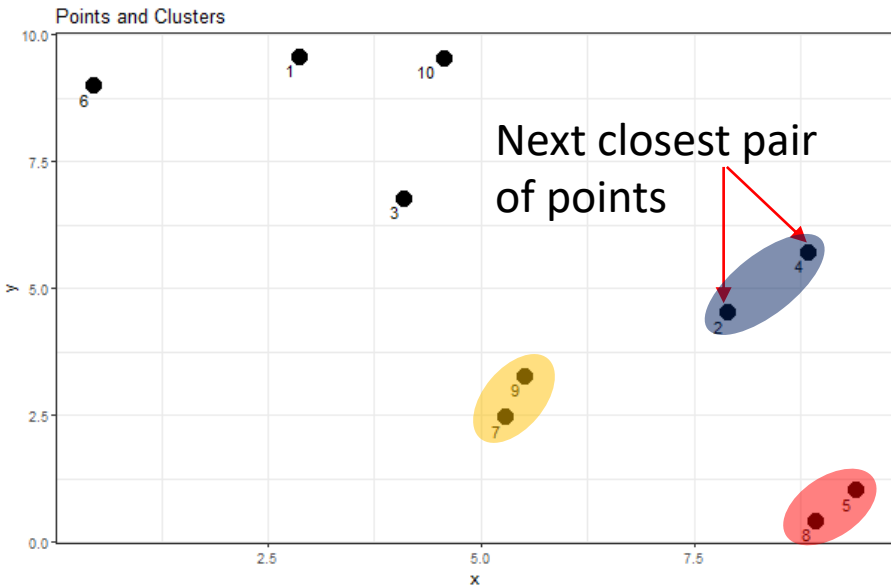


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Hierarchical Clustering

How the dendrogram is created

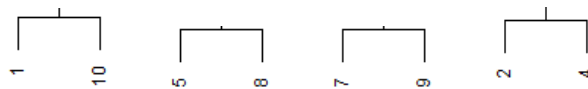
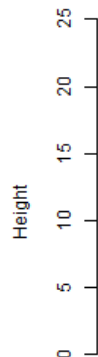
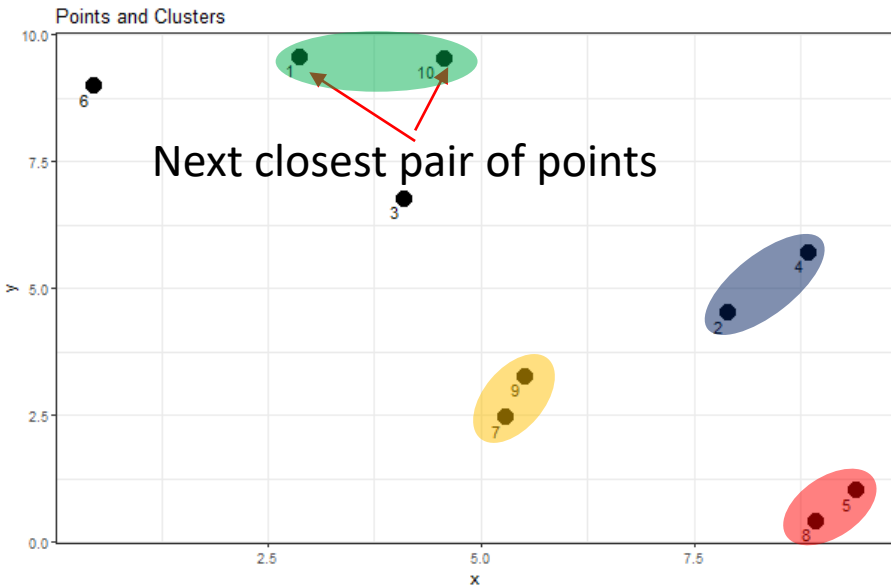
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Hierarchical Clustering

How the dendrogram is created

- Then find next closest pair of points

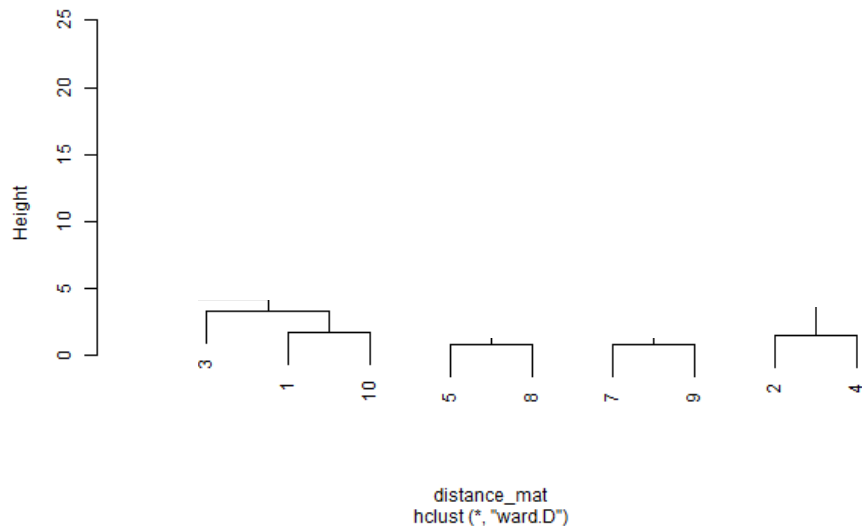
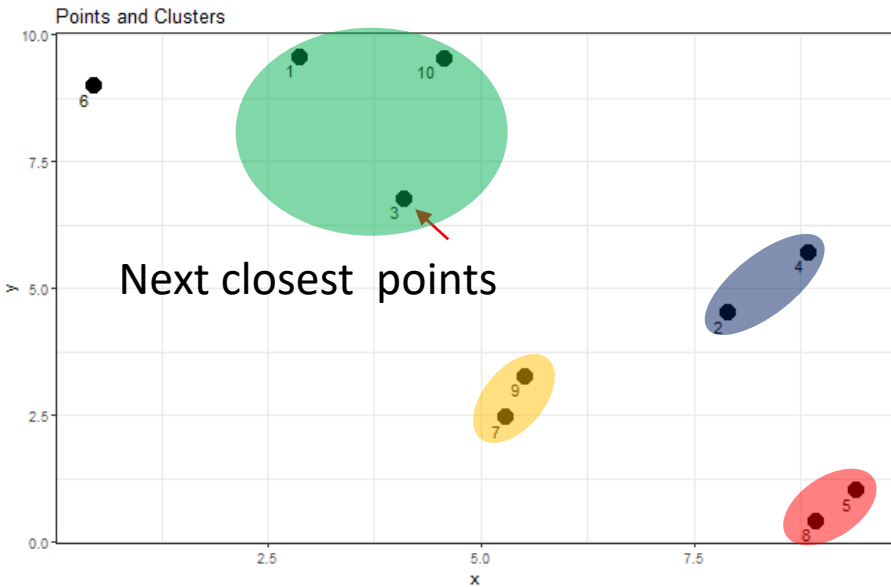


distance_mat
hclust(*, "ward.D")

Hierarchical Clustering

How the dendrogram is created

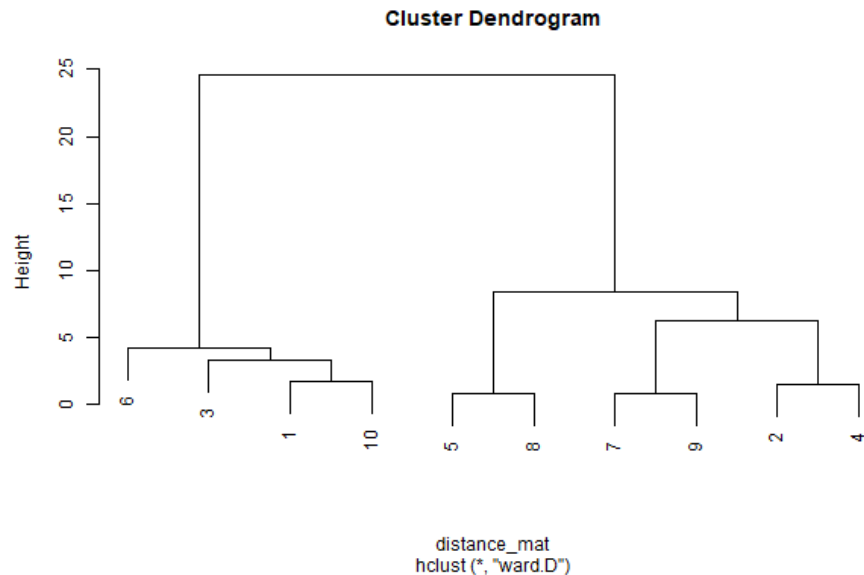
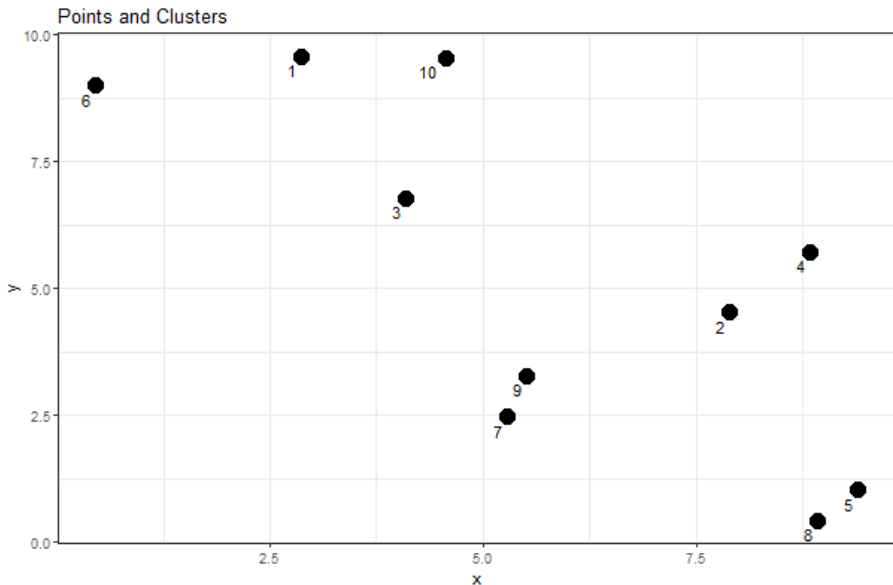
- Then find next closest pair of points



Hierarchical Clustering

How the dendrogram is created

- Finally dendrogram is created

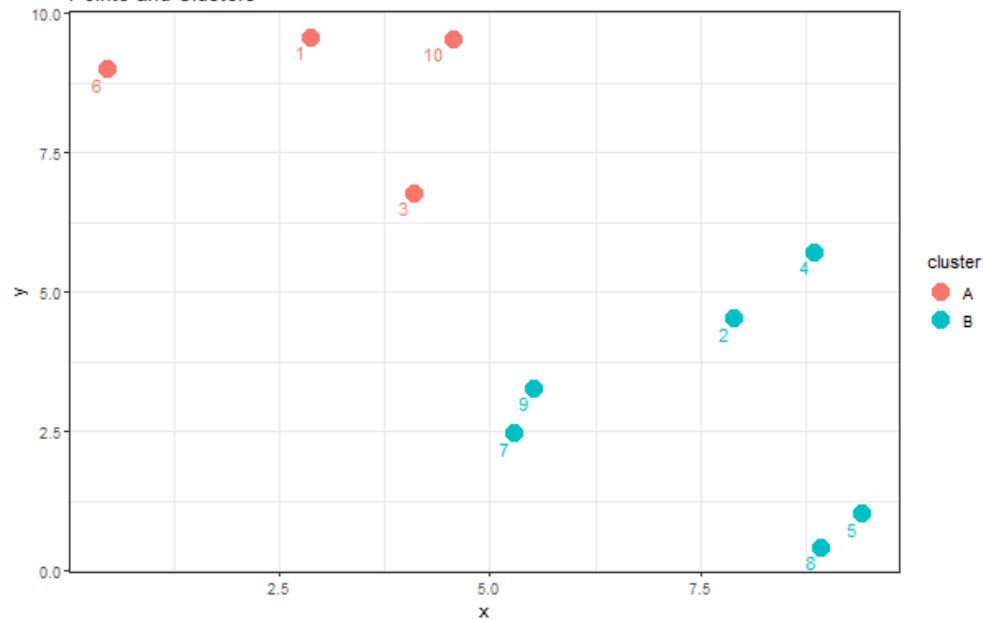


Hierarchical Clustering

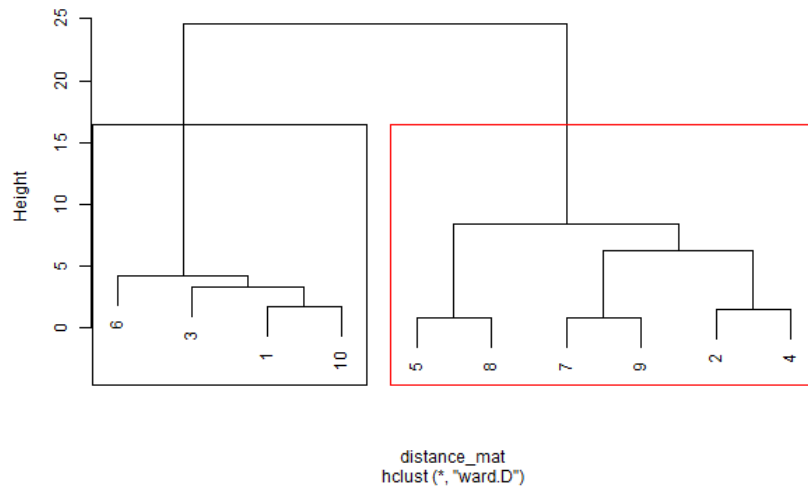
Number of Clusters

- Search longest branch, cut at the middle

Points and Clusters



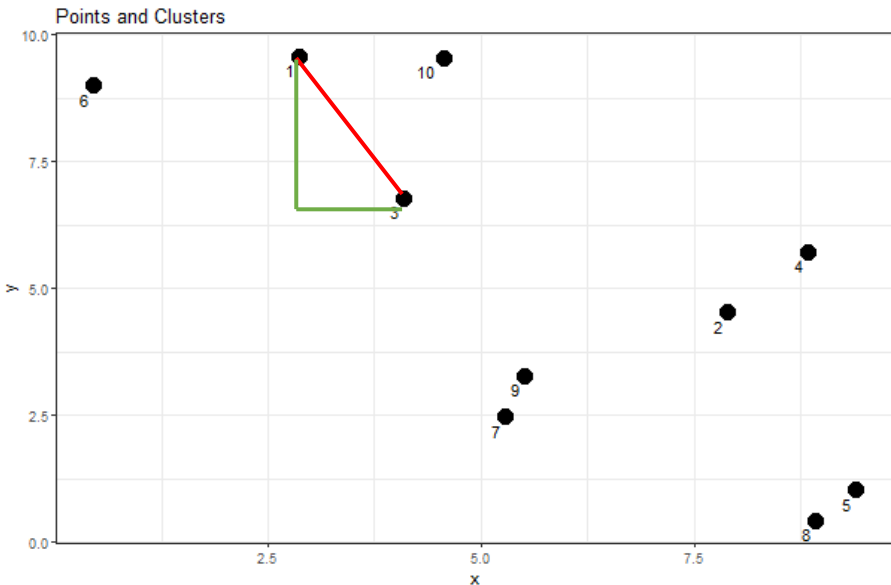
Cluster Dendrogram



Hierarchical Clustering

Distance Metrics

- Finally dendrogram is created



Most used:

- Euclidean Distance
- Manhattan Distance

Other distance metrics:

- Canberra
- Maximum
- Minkowski
- ...

Hierarchical Clustering

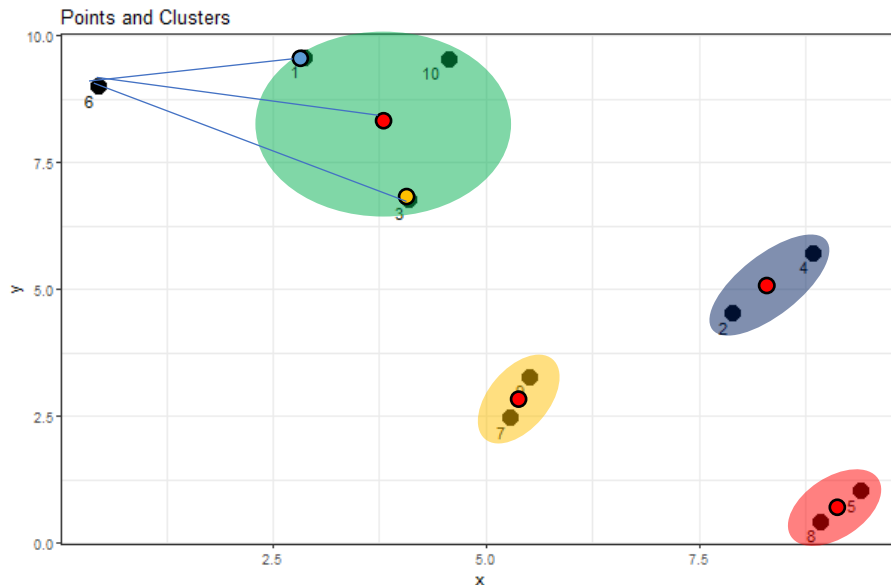
Linkage

- How to assess proximity from point / cluster to an existing cluster?

- Centroid
- Single Linkage
- Complete Linkage

Further methods:

- Ward
- Median
- Mcquitty
- ...



Hierarchical Clustering

Difference kmeans and Hierarchical Clustering

Parameter	Kmeans	HC
Complexity	$O(n)$	$O(n^2)$
Reproducibility	No	yes
Setting of Cluster Number	pre-knowledge required	No pre-knowledge required

Hierarchical Clustering

Advantages / Disadvantages



- Easy to understand
- Provides informative hierarchy
- Simpler decision on number of clusters
- User only needs to define distance metric AND linkage



- Computational effort
- Sensitive to outliers
- Sensitive to noise
- Not easily applicable for data with numerical and categorical variables
- Missing data