TECHNISCHE UNIVERSITÄT KAISERSLAUTERN

9.3 Hierarchical Clustering

Machine Learning 1: Foundations

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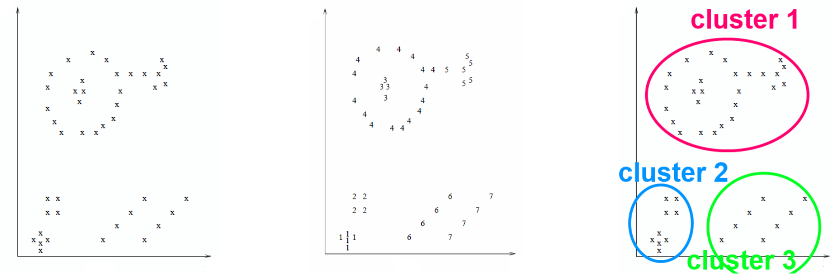
1 Linear Clustering

2 Non-linear Clustering

3 Hierarchical Clustering

Disadvantage

Big problem in *k*-means: do not know the number of clusters in advance

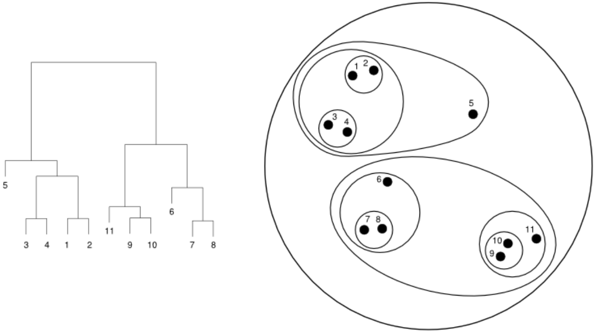


7 clusters vs. 3 clusters

What to do?

Hierarchical Clustering

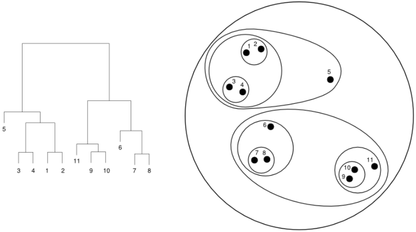
- Generates a tree ("hierarchy") of clusters



  - do not need to specify number of clusters

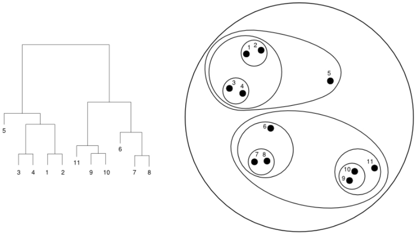
Hierarchical Clustering

function HIERARCHICALCLUSTERING(inputs $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$)
    assign each input to a cluster
    repeat
        link the two clusters with minimal distance
    until finished
    return tree of cluster linkages
end function



Hierarchical Clustering

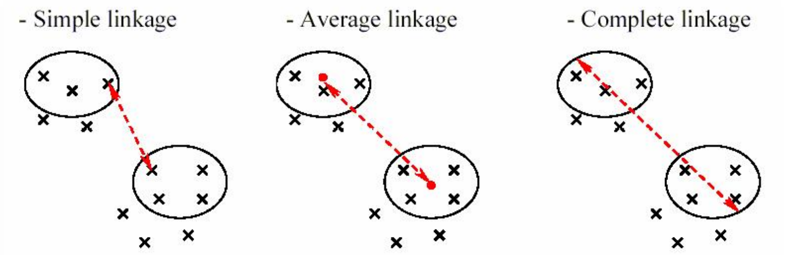
function HIERARCHICALCLUSTERING(inputs $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$)
  assign each input to a cluster
  repeat
    link the two clusters with minimal distance
  until only a single root cluster left
  return tree of cluster linkages
end function



How to measure distance between two clusters?

Hierarchical Clustering

Quiz: How to measure distance $d(i,j)$ between two clusters i and j?

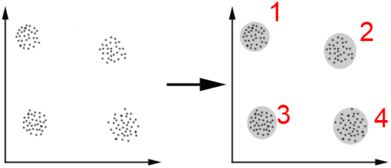


- Let $S_j \subseteq \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ be the set of inputs contained in the jth cluster
- **Simple linkage**: $d(i,j) := \min_{\mathbf{x}\in S_i, \tilde{\mathbf{x}}\in S_j} \|\mathbf{x} - \tilde{\mathbf{x}}\|$
- **Average linkage**: $d(i,j) := \operatorname{mean}_{\mathbf{x}\in S_i, \tilde{\mathbf{x}}\in S_j} \|\mathbf{x} - \tilde{\mathbf{x}}\|$
- **Complete linkage**: $d(i,j) := \max_{\mathbf{x}\in S_i, \tilde{\mathbf{x}}\in S_j} \|\mathbf{x} - \tilde{\mathbf{x}}\|$
- Note: again, all this can be kernelized...

Conclusion

Clustering:

- Organizing data into groups



k-means:

- Alternatingly, assign inputs to closest cluster center and re-compute centers
- Can be kernelized
- Can be deepified using transfer learning

Hierarchical clustering:

- Consider clusters at various scales
- Helpful when the number of clusters is unknown

Refs I