TECHNISCHE UNIVERSITÄT
KAISERSLAUTERN

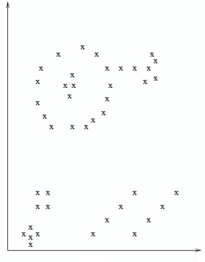
9.3 Hierarchical Clustering

Machine Learning 1: Foundations

Marius Kloft *(TUK)*

Disadvantage

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



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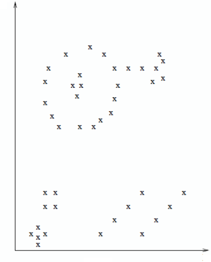

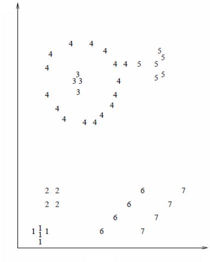

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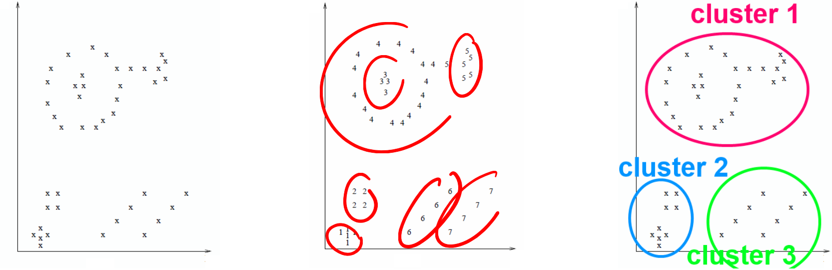

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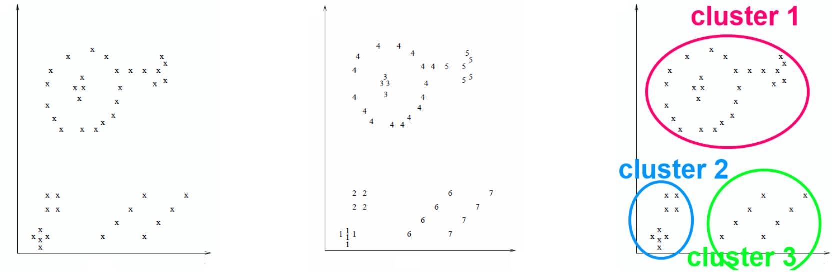

7 clusters vs. 3 clusters

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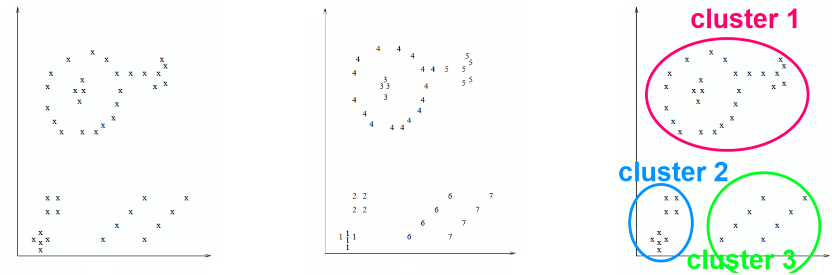


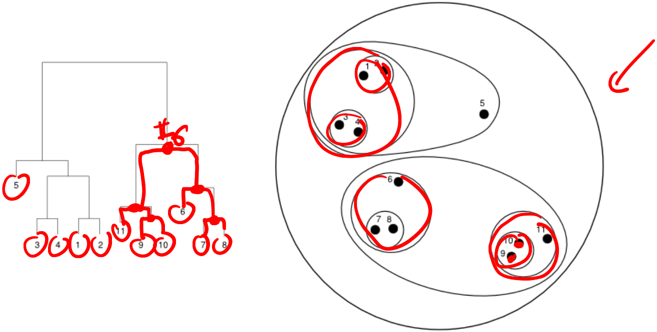
7 clusters vs. 3 clusters

Quiz: what to do?

Hierarchical Clustering

Hierarchical Clustering

- Generates a tree (“hierarchy”) of clusters



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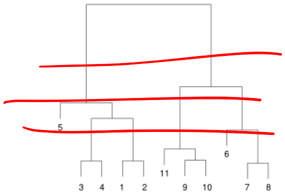

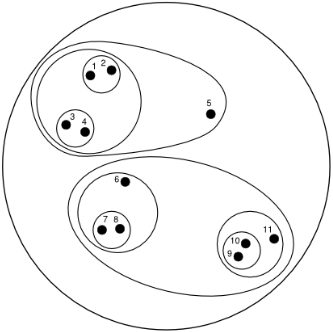

  - do not need to specify number of clusters

Hierarchical Clustering

1: **function** HIERARCHICALCLUSTERING(inputs $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$)

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function HIERARCHICALCLUSTERING(inputs $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$)
    assign each input to a cluster

Hierarchical Clustering

```
function HIERARCHICALCLUSTERING(inputs x_1, ..., x_n ∈ ℝ^d)
    assign each input to a cluster
    repeat
        link the two clusters with minimal distance
```

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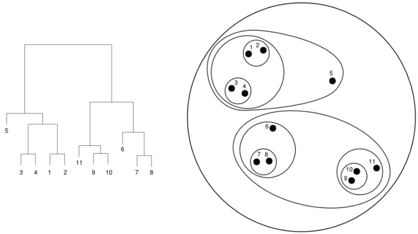

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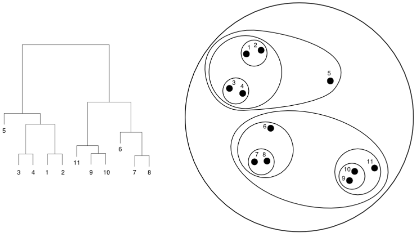

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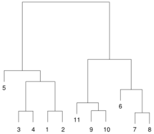

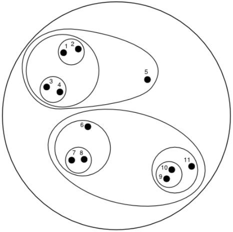

How to measure distance between two clusters?

Hierarchical Clustering

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

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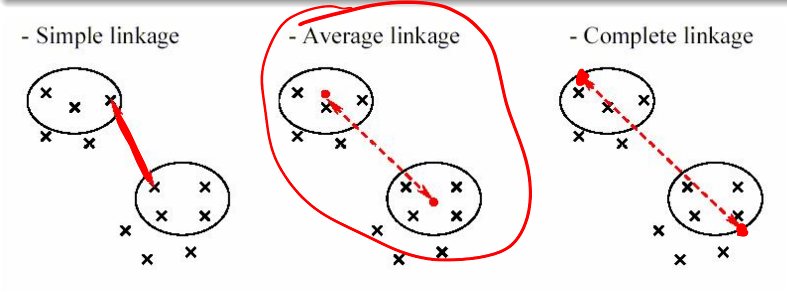

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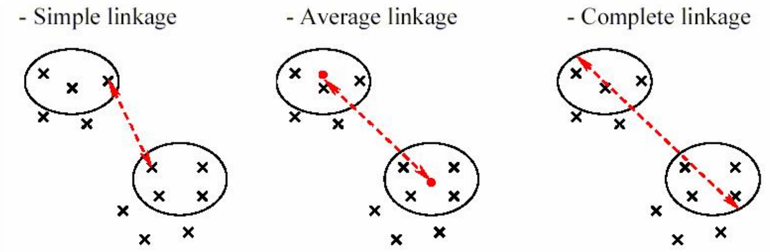

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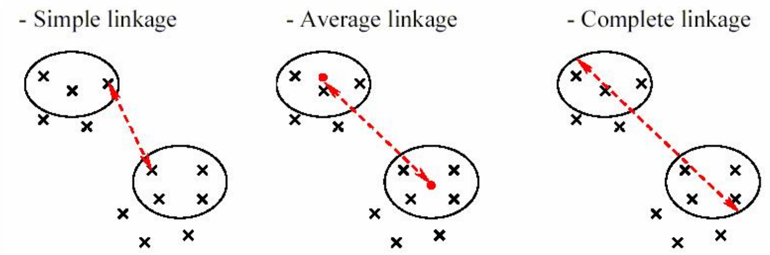

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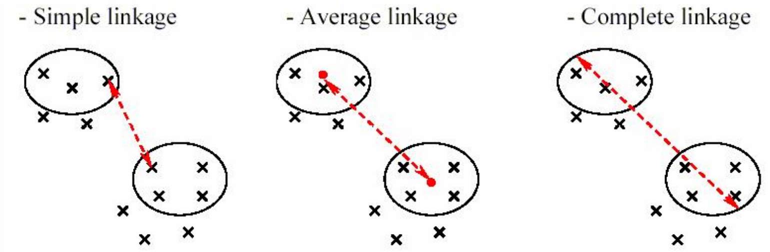

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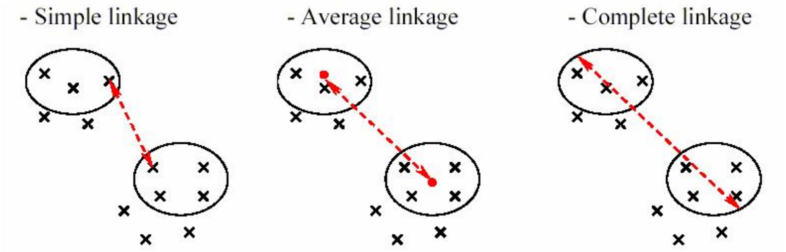

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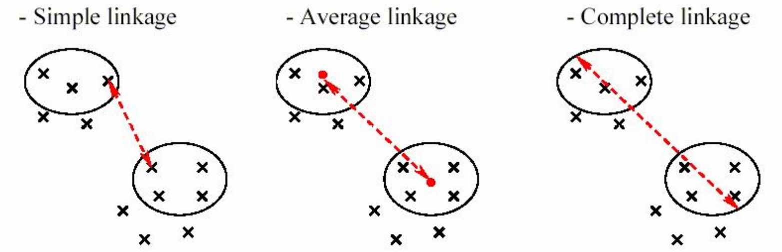

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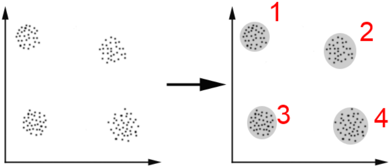
- Note: again, all this can be kernelized...

Conclusion

Clustering:

- Organizing data into groups



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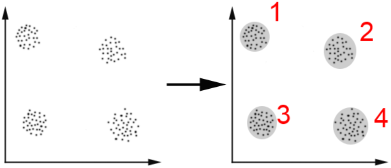

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- Alternatingly, assign inputs to closest cluster center and re-compute centers

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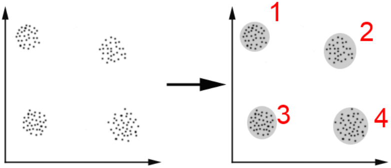

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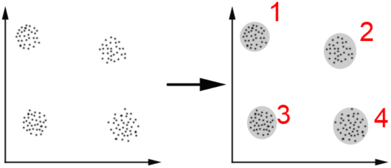

k-means:

- 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