https://github.com/tedinburgh/ads2023

Clustering: Hierarchical clustering

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Example classes and lecture notes

- There are 2 more small group classes, this week and the following week
- You should know the group/time/room, please email me (te269) or Steven (stg20) if not
- This week's problem set: decision trees
  - Chapter 8 of Introduction to Statistical Learning with Python
  - Questions 4, 5, 9, 10 (extension Q12, ignore BART)
  - Pdf of the book and .csv files available at https://www.statlearning.com/
- Notes covering the first half of the course will be online on the Moodle soon

Clustering schedule

1. k-means
2. Hierarchical clustering
3. Gaussian mixture models, self-organising maps, spectral clustering
4. Graph-based clustering, density-based clustering, outlier detection
5. Clustering evaluation, hyperparameters, pros and cons, consensus clustering

Today: hierarchical clustering

- Overview
- Hierarchical agglomerative clustering
- Linkage
- Code example (k-means and hierarchical clustering)
- Vector quantisation

Questions: halfway through, at the end, or by email (te269)

Resources

- Introduction to Statistical Learning with Python, Chapter 12

- Slides adapted from:
  - Prof Stephen Eglen, Cambridge
  - Ethan Fetaya/James Lucas/Emad Andrews, Toronto
  - Ronan Cummins, Cambridge

Overview: hierarchical clustering

- Build a hierarchy of clusters
- Small clusters have parents
- Agglomerative (bottom-up) vs divisive (top-down)
- Some similarities and some differences to decision trees (supervised learning)
- We don’t even really need to know the observations themselves, a matrix of distances is enough
- Hierarchical clustering results in a sequence of clusters

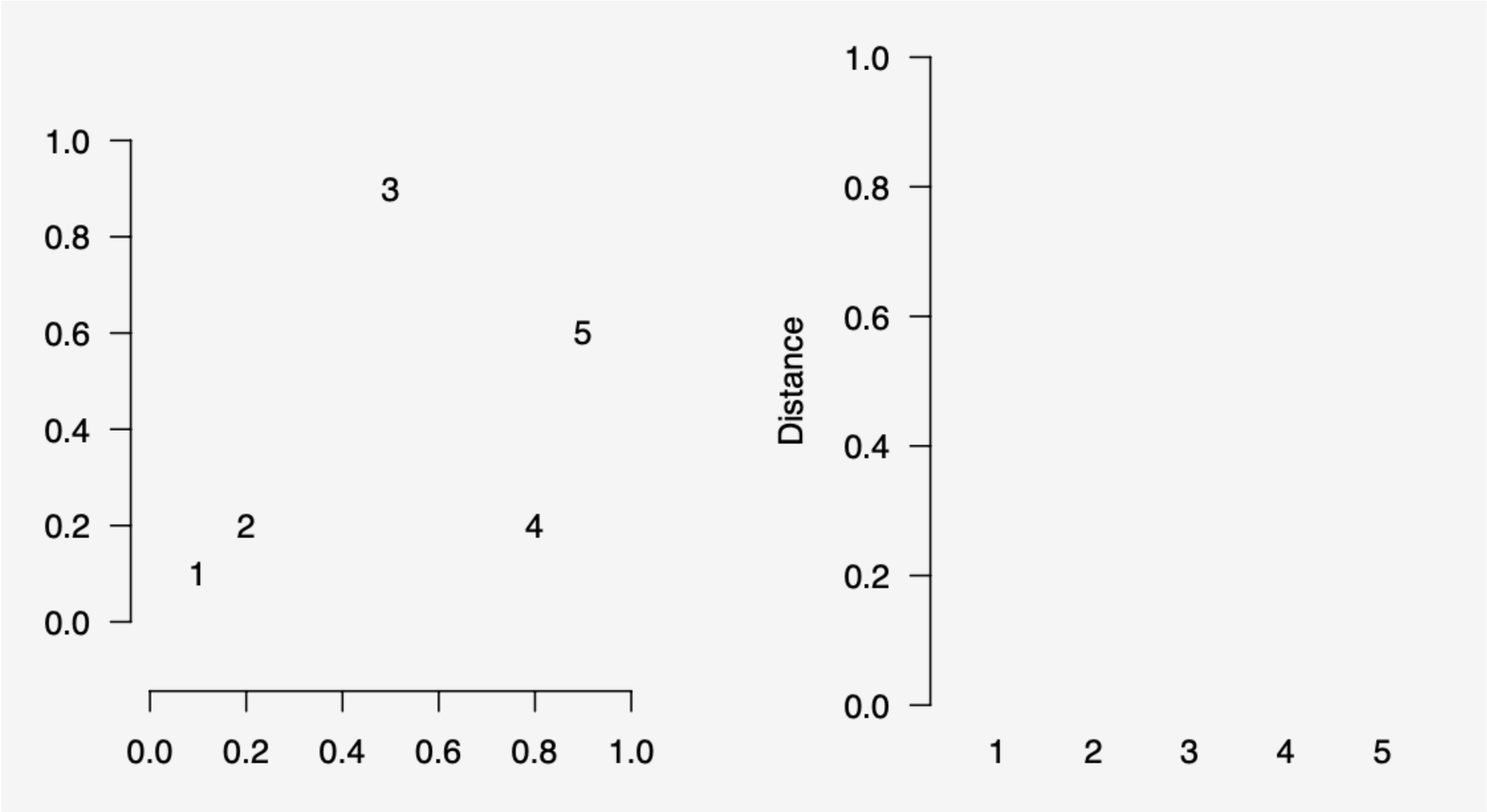
One cluster per observation ⟷ One cluster with all observations

Hierarchical agglomerative clustering

- Start with each observation in its own separate cluster
- Merge the two clusters that are the most similar
- Repeat until there is only one cluster with all observations (greedy)
- The history of how clusters merged forms a binary tree called a dendrogram

- We need a way to describe the similarity between clusters
  - Lots of similarity/dissimilarity measures

Example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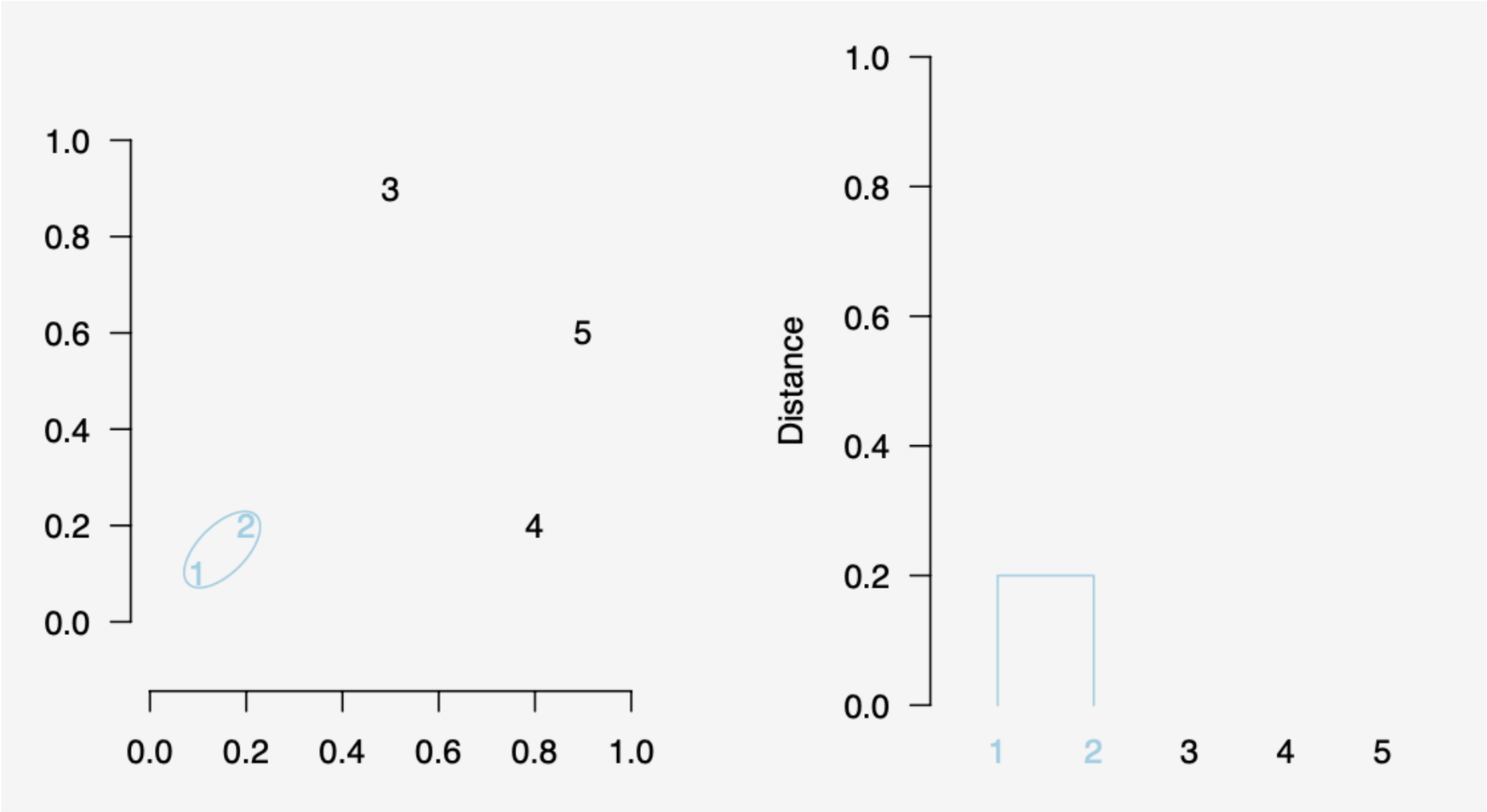
Example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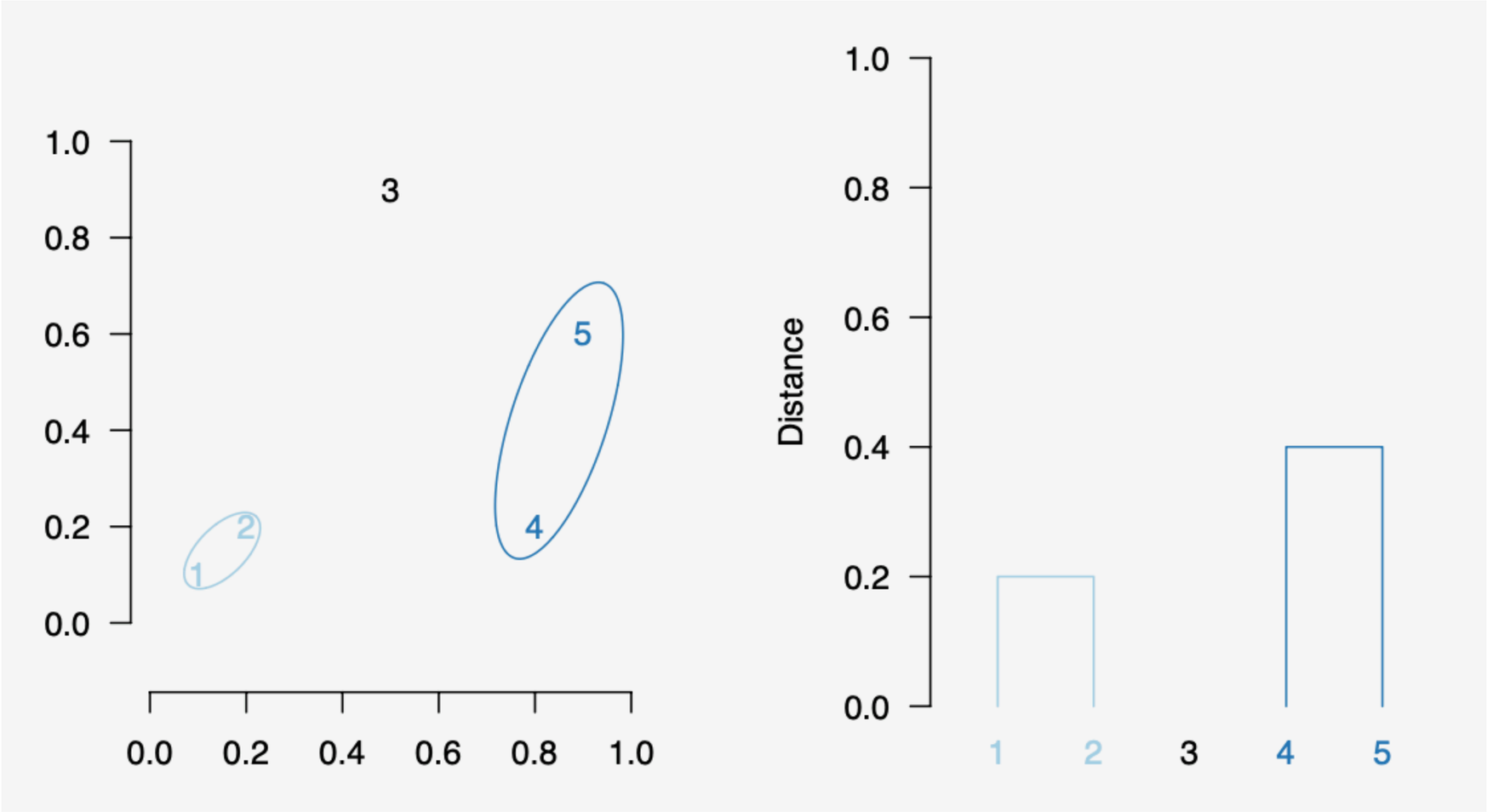
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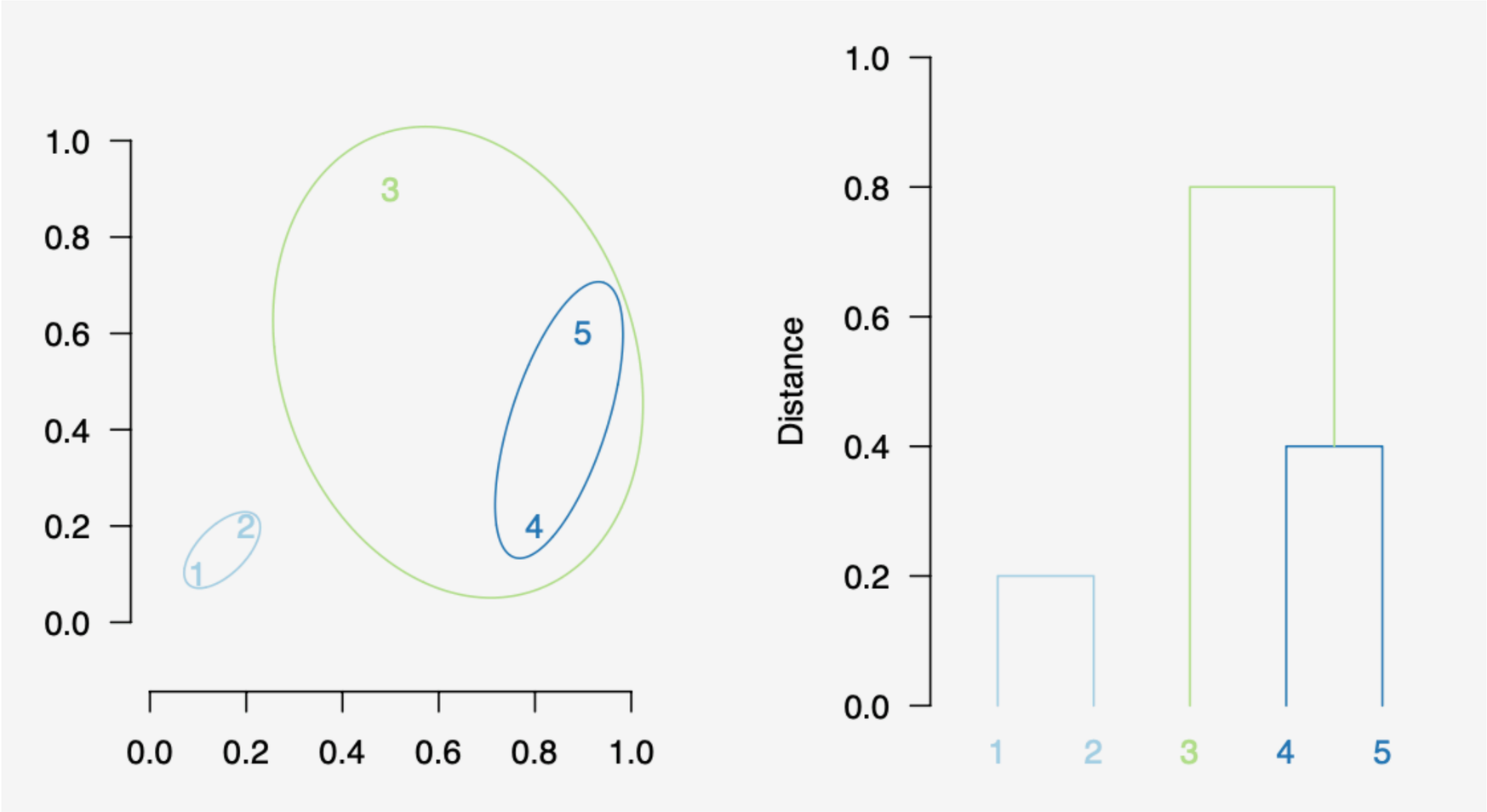
Example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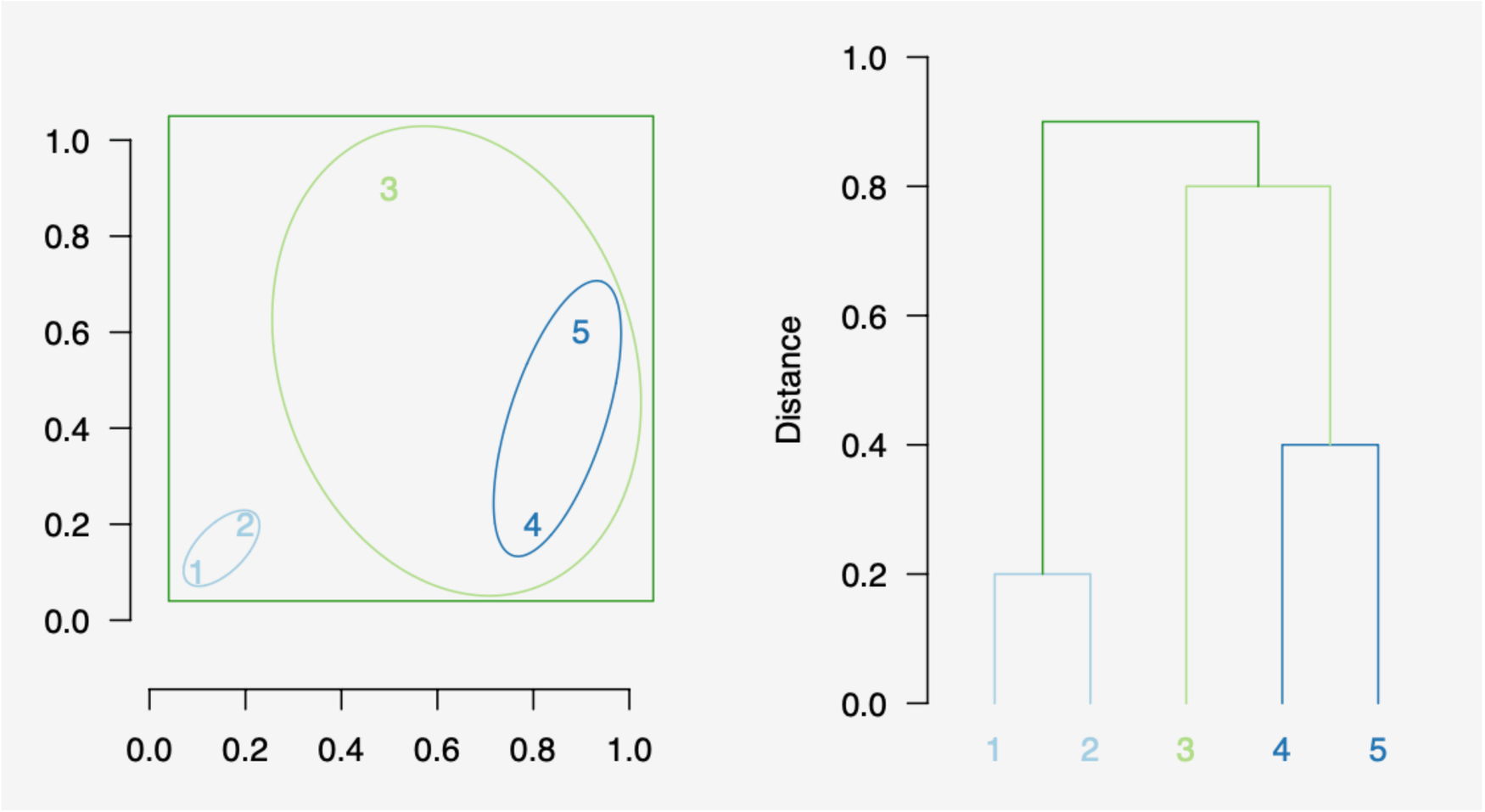
Example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Distance
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Linkage

- The linkage is a similarity function between clusters (not observations)
- Lots of options, e.g.
  - Single linkage: distance between closest observations in each cluster
  - Complete linkage: distance between furthest observations in each cluster
  - Average linkage: average distance between each pair of observations
  - Centroid linkage: distance between cluster centroids
  - Ward linkage: minimum increase in sum of squares distance from centroids

Single linkage, complete linkage and average linkage

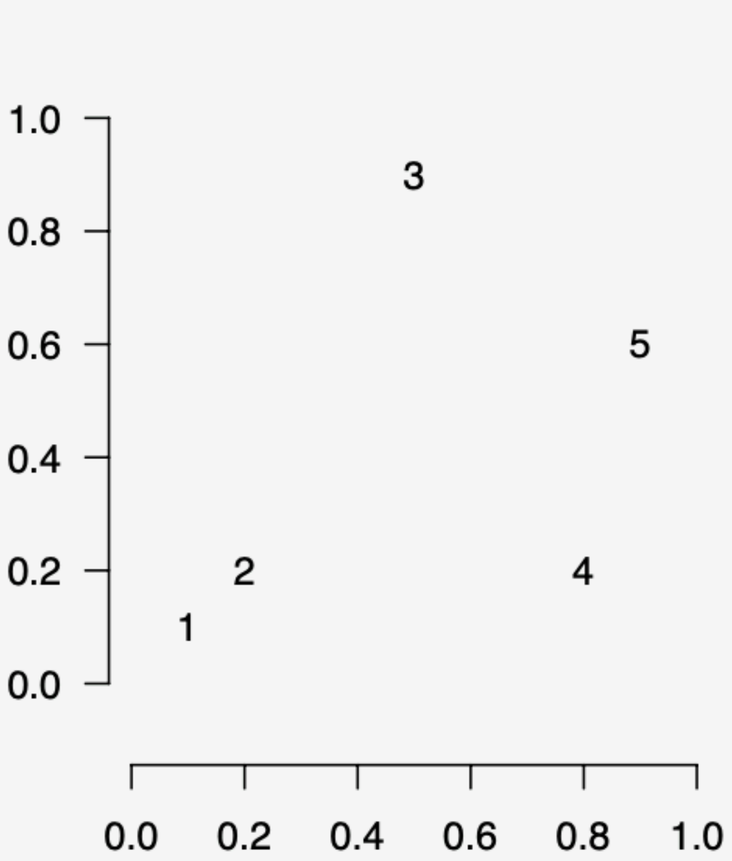
- Notation: cluster set A contains $n_A = |A|$ and has centroid $c_A = 1/n_A \sum_{x \in A} x$. Then:
  - Single linkage: $d(A, B) = \min_{x \in A, y \in B} d(x, y)$
  - Complete linkage: $d(A, B) = \max_{x \in A, y \in B} d(x, y)$
  - Average linkage: $d(A, B) = 1/(n_A n_B) \sum_{x \in A} \sum_{y \in B} d(x, y)$

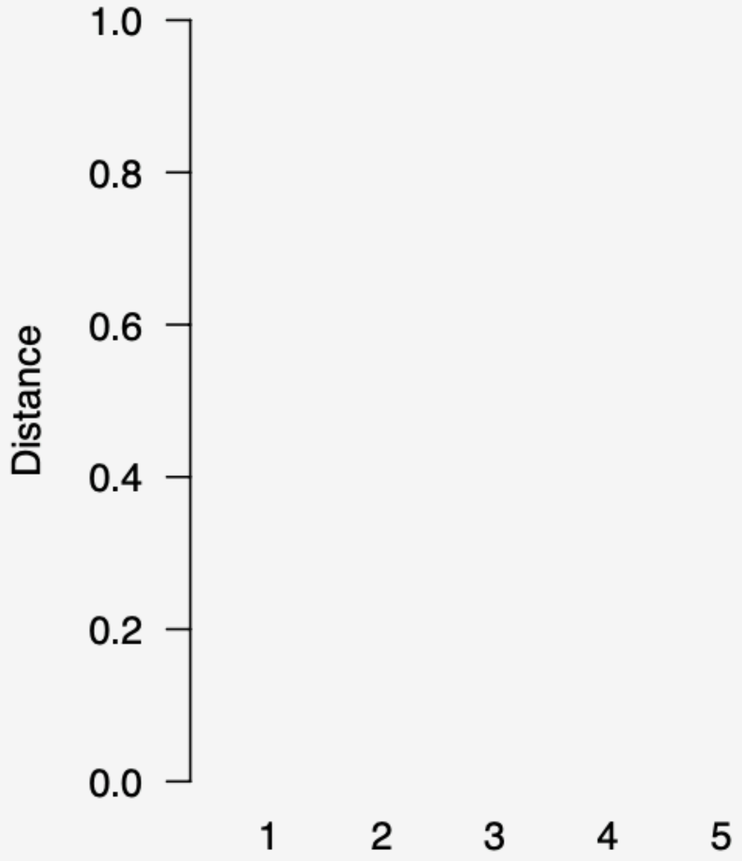
Centroid linkage and Ward linkage

- Notation: cluster set A contains $n_A = |A|$ and has centroid $c_A = 1/n_A \sum_{x \in A} x$. Then:
  - Centroid linkage: $d(A, B) = \|c_A - c_B\|^2$
  - Ward linkage: $d(A, B) = \sum_{x \in A \cup B} \|x - c_{A \cup B}\|^2 - \sum_{x \in A} \|x - c_A\|^2 - \sum_{x \in B} \|x - c_B\|^2$

Example (centroid linkage)

d	2	3	4	5
1	0.2	1.1	0.9	1.1
2		0.9	0.7	0.8
3			0.7	0.5
4				0.4





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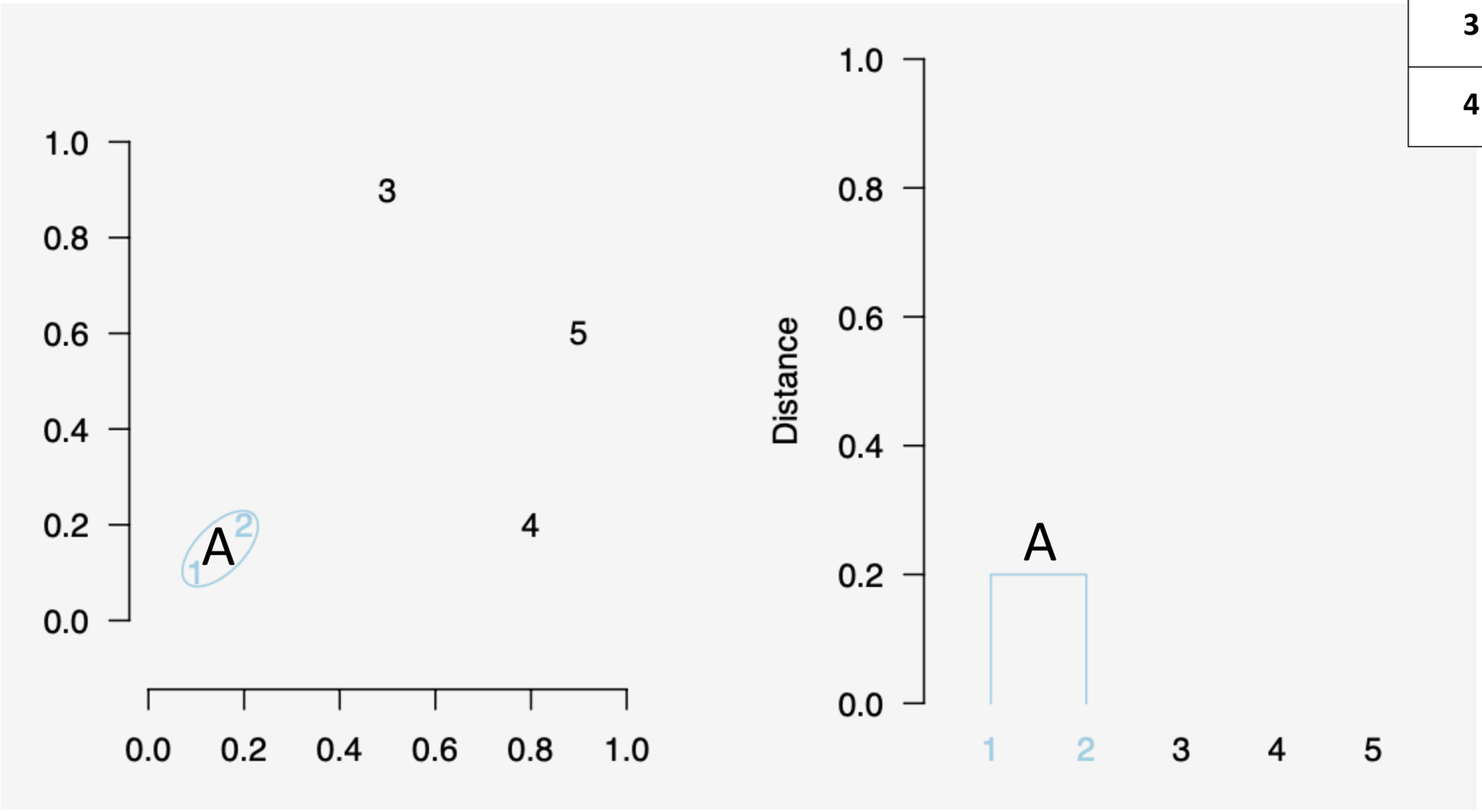
1	0.2	1.1	0.9	1.1
2		0.9	0.7	0.8
3			0.7	0.5
4				0.4

d	3	4	5
A	1.0	0.6	0.9
3		0.7	0.4
4			0.3



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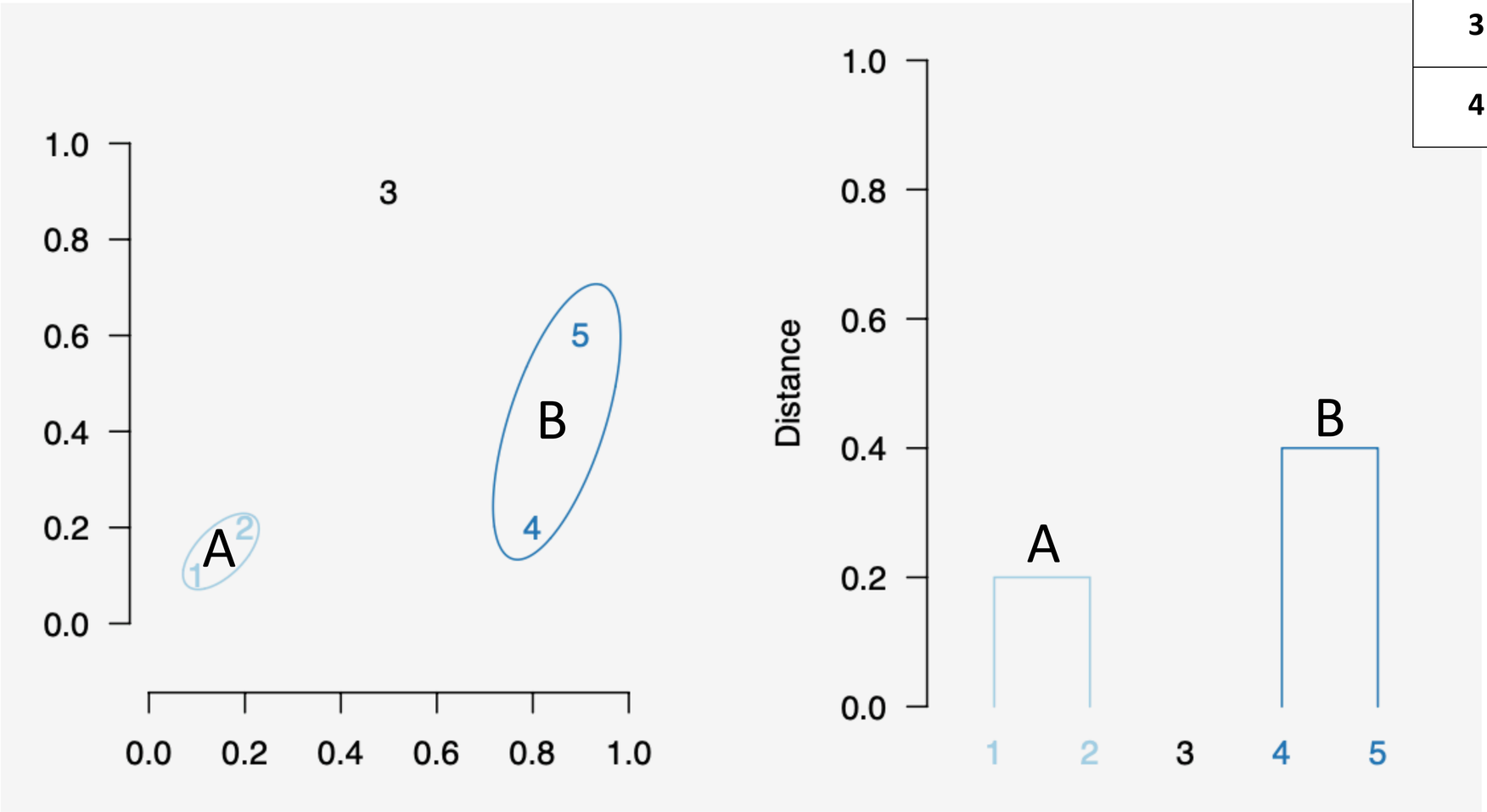

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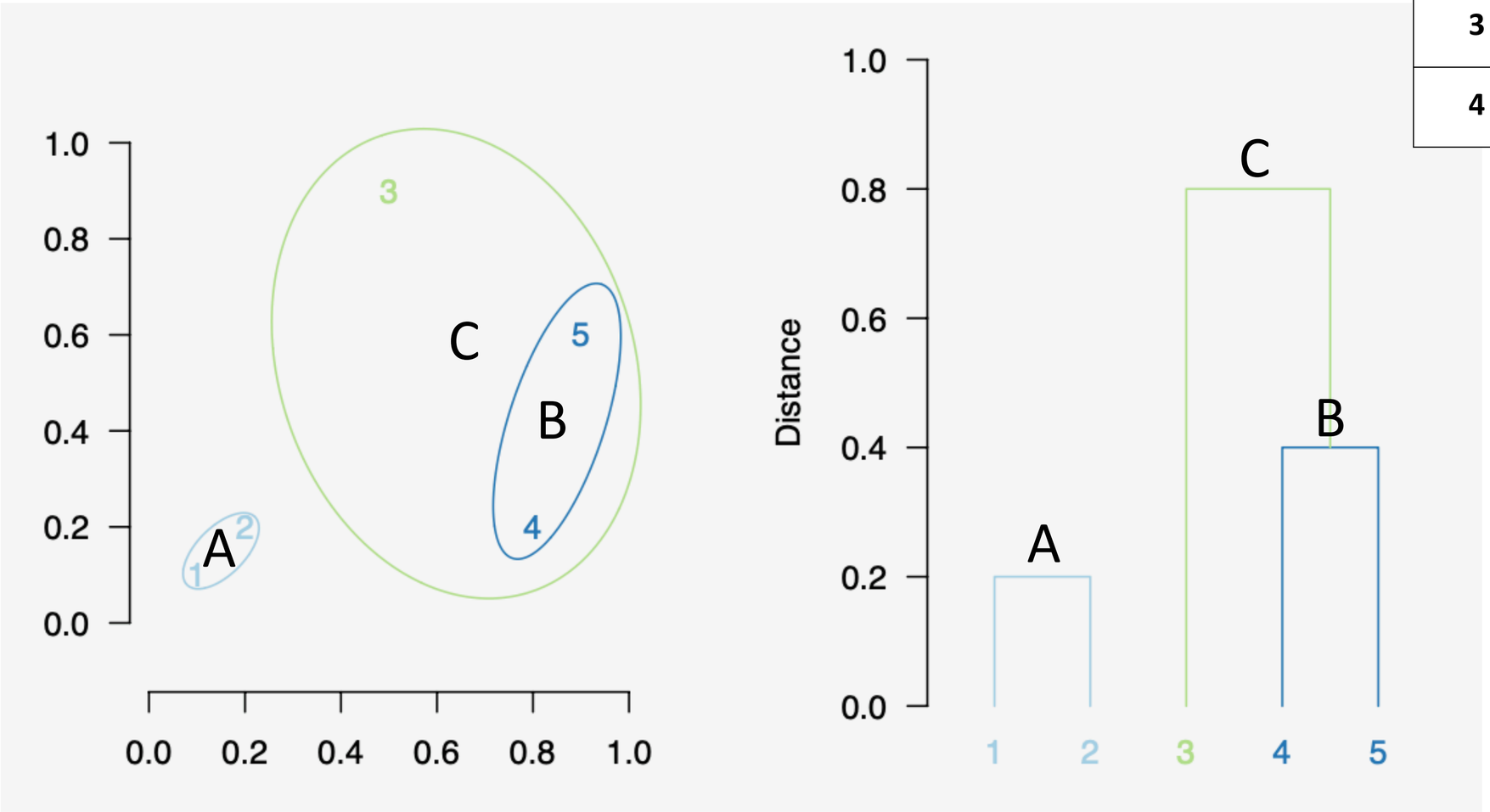
2		0.9	0.7	0.8
3			0.7	0.5
4				0.4

d	3	4	5
A	1.0	0.6	0.9
3		0.7	0.4
4			0.3

d	3	B
A	1.0	0.7
3		0.4

Example (centroid linkage)



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4				0.4

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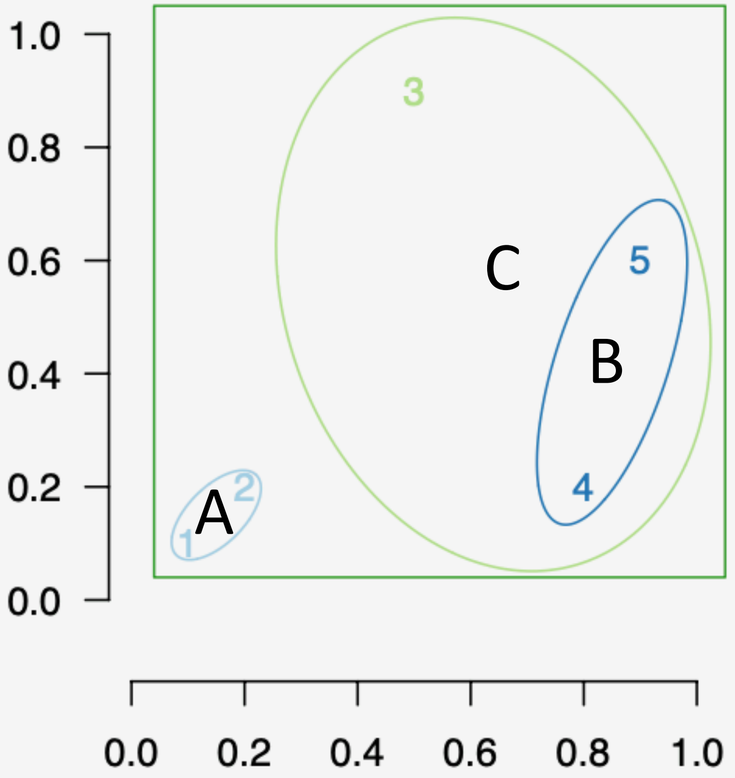
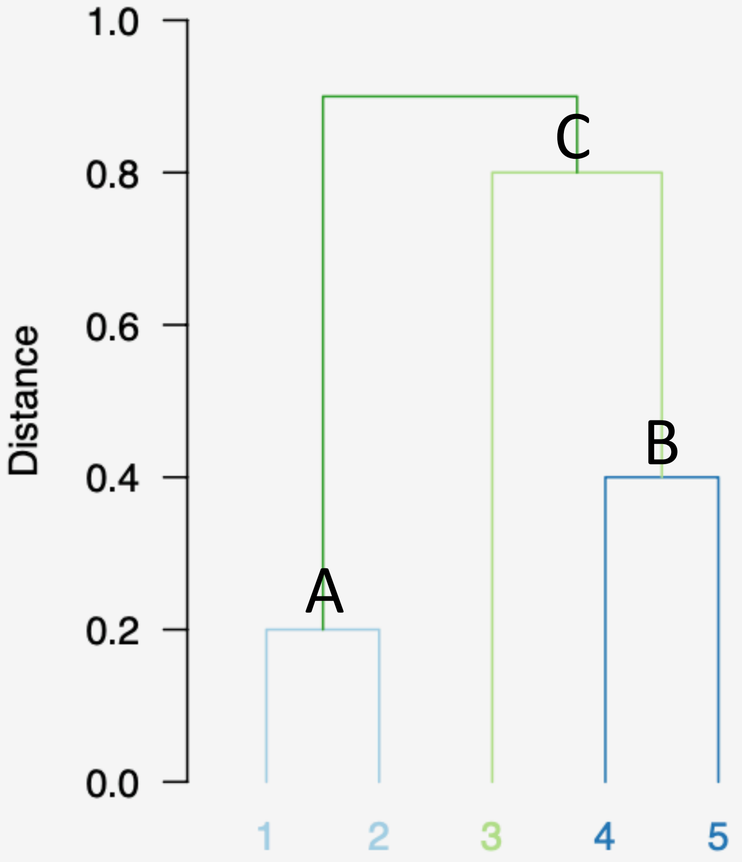
A	1.0	0.6	0.9
3		0.7	0.4
4			0.3

d	3	B
A	1.0	0.7
3		0.4

d	C
A	0.7

Example (centroid linkage)





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3		0.7	0.4
4			0.3

d	3	B
A	1.0	0.7
3		0.4

d	C
A	0.7

Linkage: some less common options

- Weighted average linkage: $d(A, B \cup C) = (d(A, B) + d(B, C))/2$
- Minimum increase in variance: $d(A, B) = \text{var}(A \cup B) - \text{var}(A) - \text{var}(B)$, $\text{var}(A) = 1/n_A \sum_{x \in A} \|x - c_A\|^2$
- Mini-max linkage: $d(A, B) = \min_{x \in A \cup B}(\max_{y \in A \cup B} d(x, y))$
- Hausdorff linkage: $d(A, B) = \max(\max_{x \in A} \min_{y \in B} d(x, y), \max_{y \in B} \min_{x \in A} d(x, y))$

J Am Stat Assoc. 2011; 106(495): 1075–1084.
doi: 10.1198/jasa.2011.tm10183

Hierarchical Clustering With Prototypes via Minimax Linkage

Jacob Bien, Ph.D. Student and Robert Tibshirani, Professor

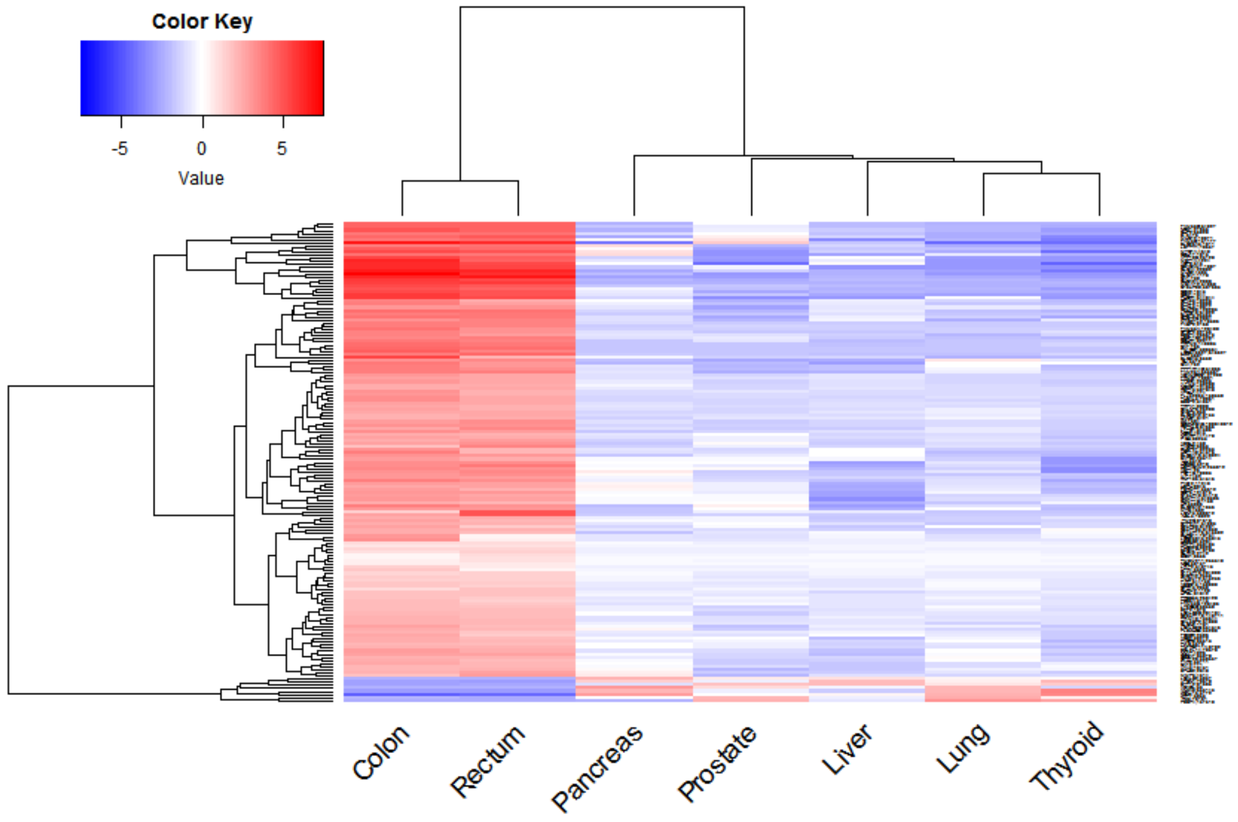
Questions?

Code example

- Jupyter notebook about hierarchical clustering
- On GitHub (https://github.com/tedinburgh/ads2023), Moodle, and course GitLab

Dendrogram

- How should we plot the dendrogram? For the same sequence of clusters, there are lots of orderings along the x-axis (2^{n-1} orderings for n observations)
- Nearby leaves are not necessarily similar
- Can affect visualisation/interpretation!
- There are some heuristics for this
  - GW method
  - Optimal leaf ordering (OLO)



Hierarchical divisive clustering

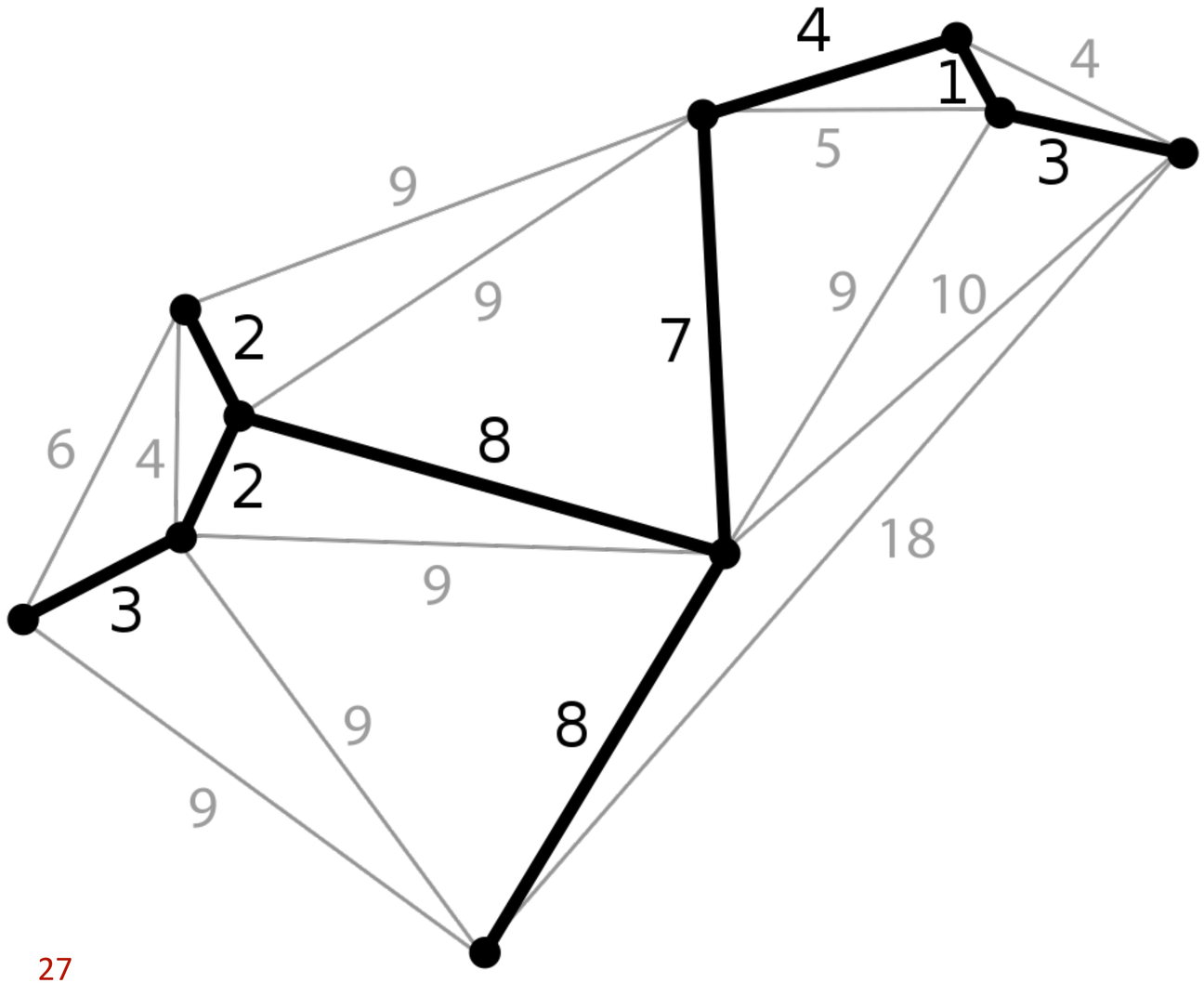
- Basic algorithm is DIANA (divisive analysis clustering)
- Start with all data in the same cluster
- At each iteration, choose one existing cluster (with the largest diameter) and build a new ‘splinter group’ nested cluster inside it
- Observations within the larger cluster can migrate to the new nested cluster
- The existing cluster gets ‘hollowed out’ as loose observations within it move into nested clusters (as more nested clusters are created)
- The nested ‘splinter group’ clusters are children of the existing cluster (compared to creating parent clusters for agglomerative clustering)

Computational complexity

- Calculate the distance between each pair of observations ($n \times n$), so $O(n^2)$, which is expensive if there are a lot of observations
- Single linkage: for n iterations, find the minimum distance (sort operation, $O(n \log n)$), overall $O(n^2) + O(n \times n \log n) = O(n^2 \log n)$
- Exhaustive search e.g. for divisive clustering $O(2^n)$
- Optimised algorithms e.g. SLINK/CLINK are $O(n^2)$ (doesn't calculate distance matrix)

Single linkage and minimum spanning trees

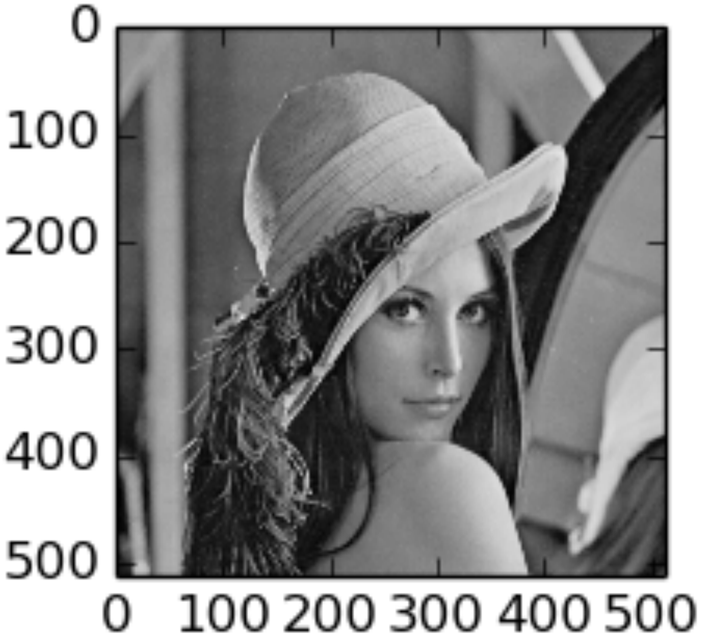
- The naïve algorithmic approach for single linkage clustering is essentially the same as Kruskal's algorithm for minimum spanning trees
- This finds the minimum distance connecting all vertices of an undirected edge-weighted graph
- Faster algorithms for single-linkage HAC correspond to more efficient algorithms for MSTs

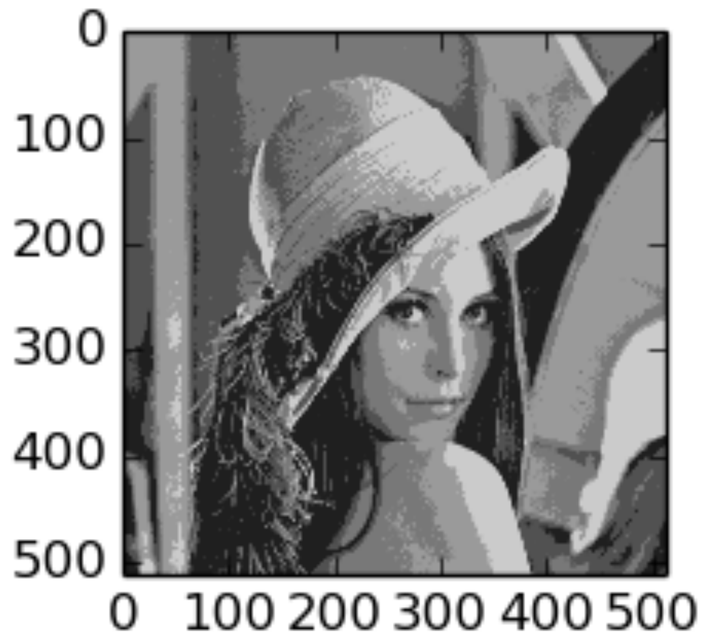


https://scikit-learn.org/0.15/auto_examples/cluster/plot_lena_compress

Vector quantisation

- Split a high-dimensional input (e.g. an image) into smaller chunks
- Perform clustering on the smaller chunks
- Replace each chunk with a representation/exemplar for that cluster (usually the centroid or medoid)
- Effectively, choose a smaller set of points to represent a larger set of points
- Useful for lossy data compression (e.g. MPEG, a precursor to JPEG)





Questions?

- Feel free to email me at te269@cam.ac.uk

Next time

- Clustering
  - Gaussian mixture models and Expectation-Maximisation
  - Self-organising maps
  - Spectral clustering