Introduction to Clustering

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What is Clustering?

"Clustering" is a broad term for algorithms in statistics and machine learning that try to discover "natural groups" in data.

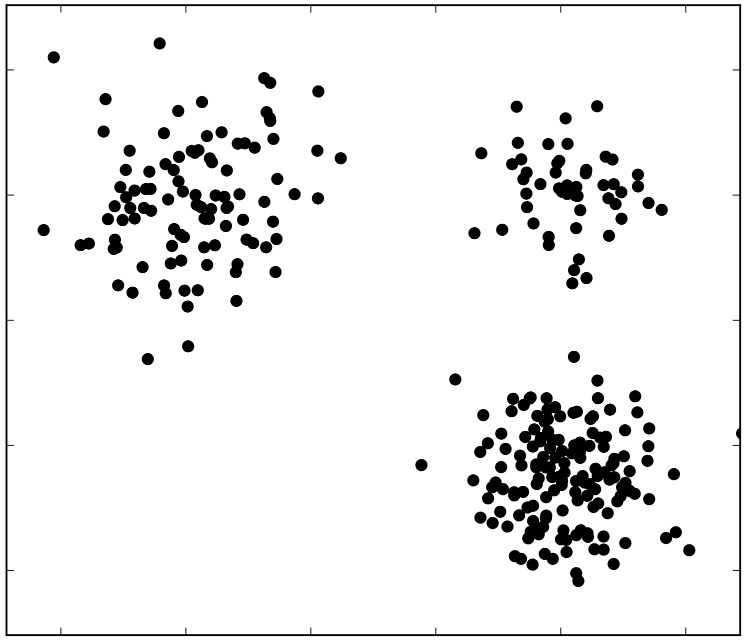
What's a "natural group"?

- Common sense definition: Groups of objects (or variables) where similarity between objects is higher within groups than between groups

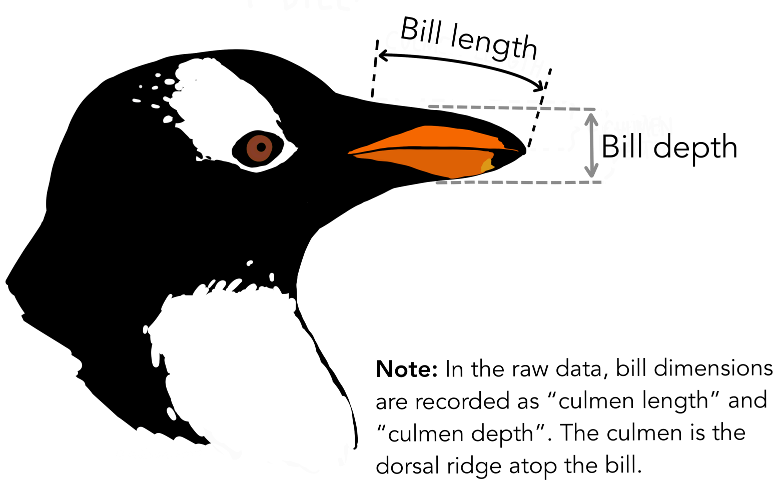
Natural Groups: Geometric Perspective

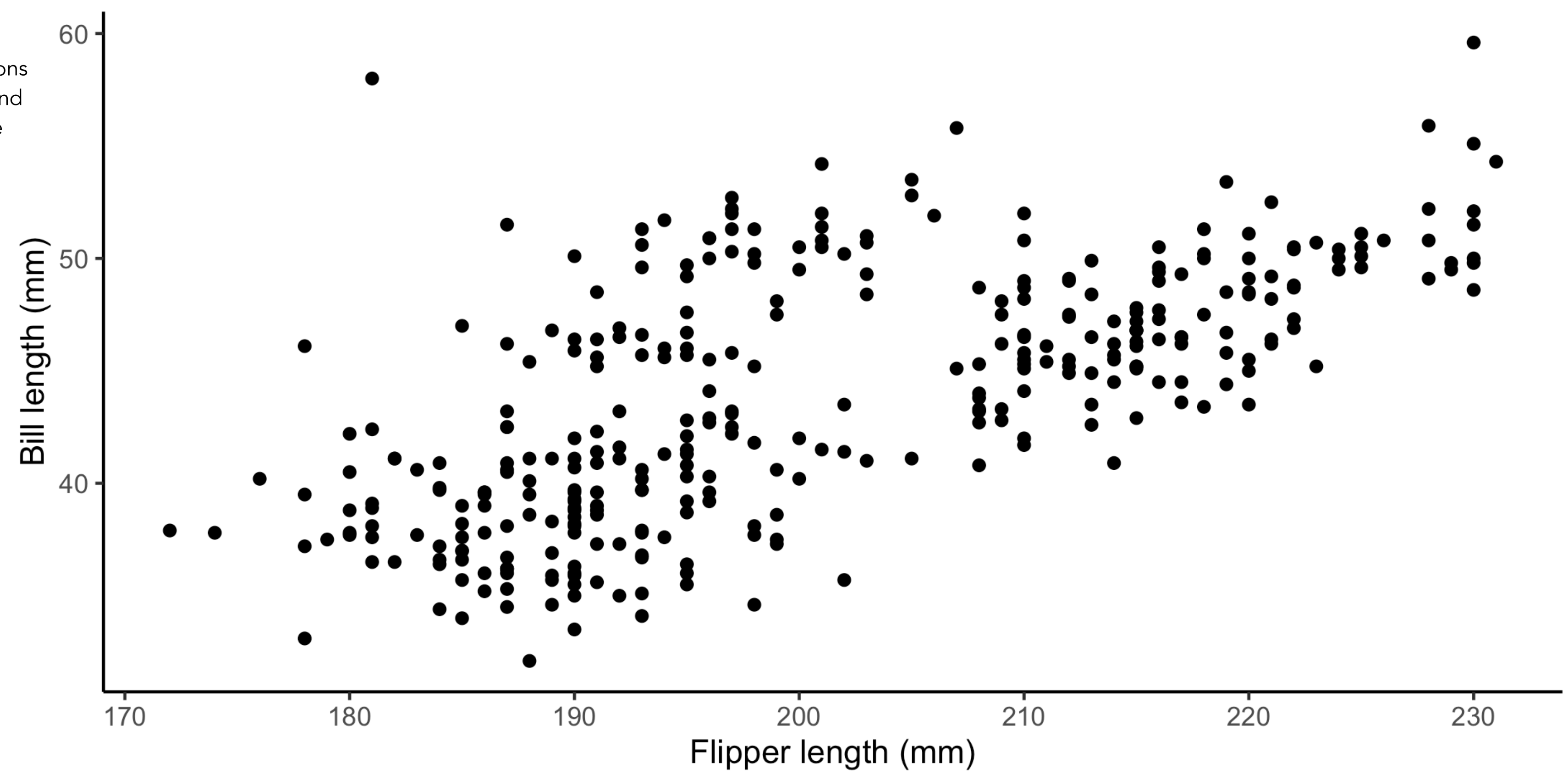
What's a "natural group"?

- Geometric definition: Patches of high density points surrounded by patches of lower density in the p-dimensional space defined by the variates.



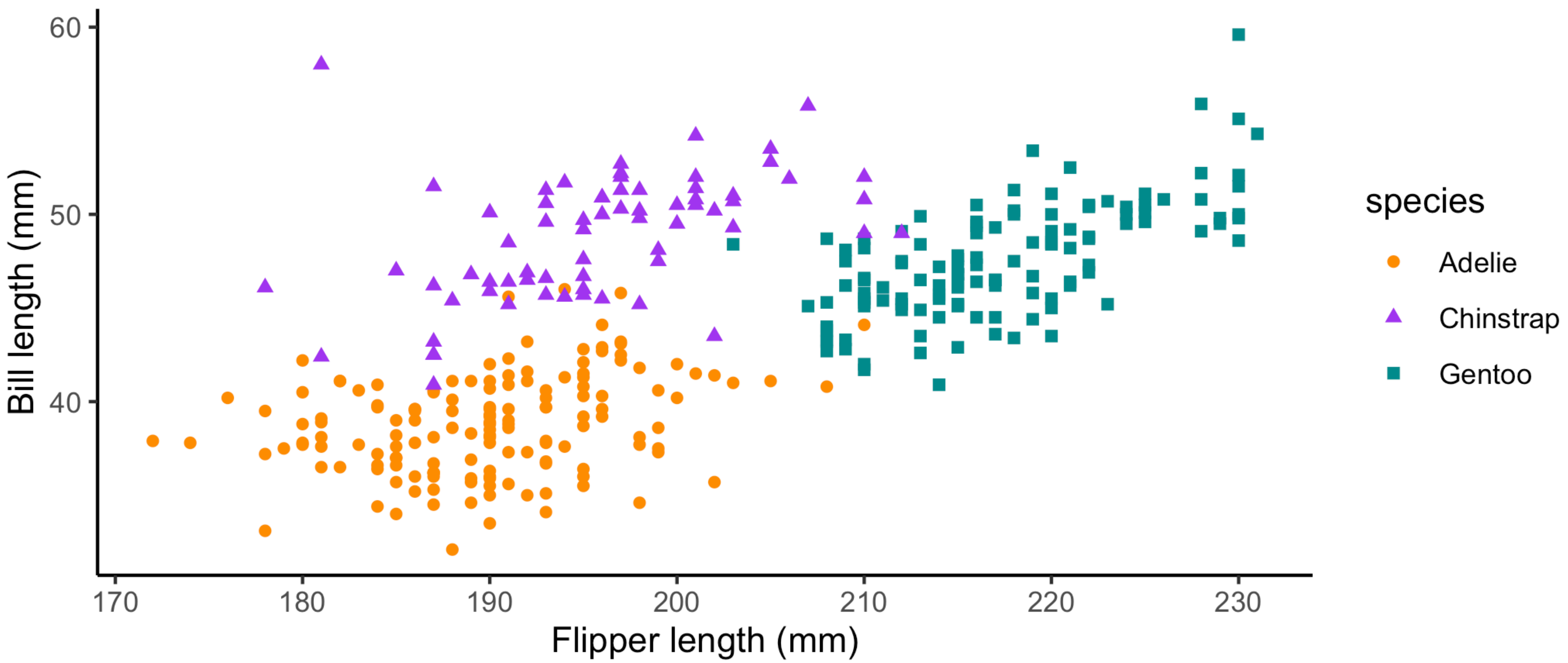
How many groups are there in this data?



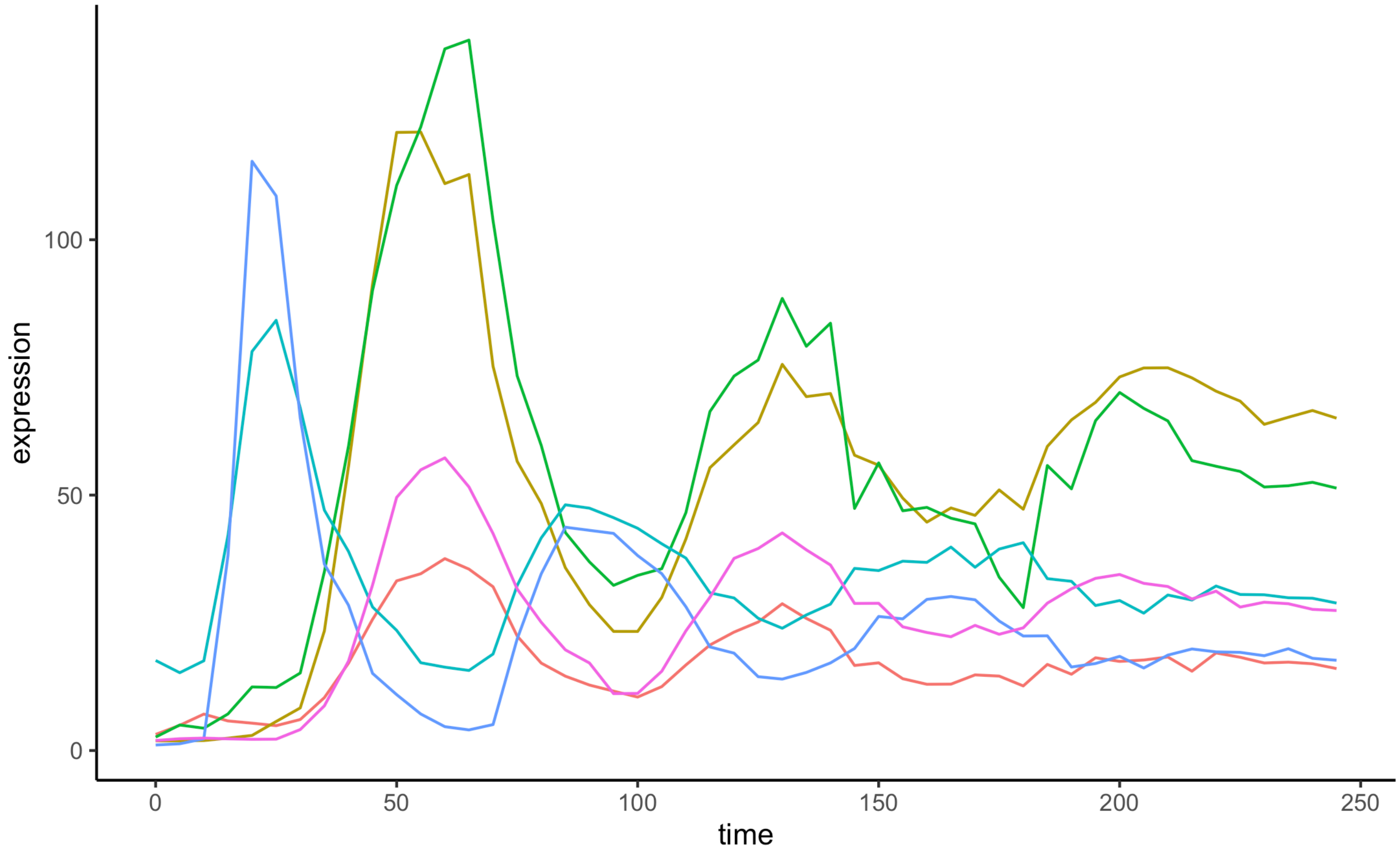


Data and images from the palmerpenguins R library (https://allisonhorst.github.io/palmerpenguins/)

Clusters based on biological data often convey useful information on biological groupings



The data used in clustering is often high dimensional and complex



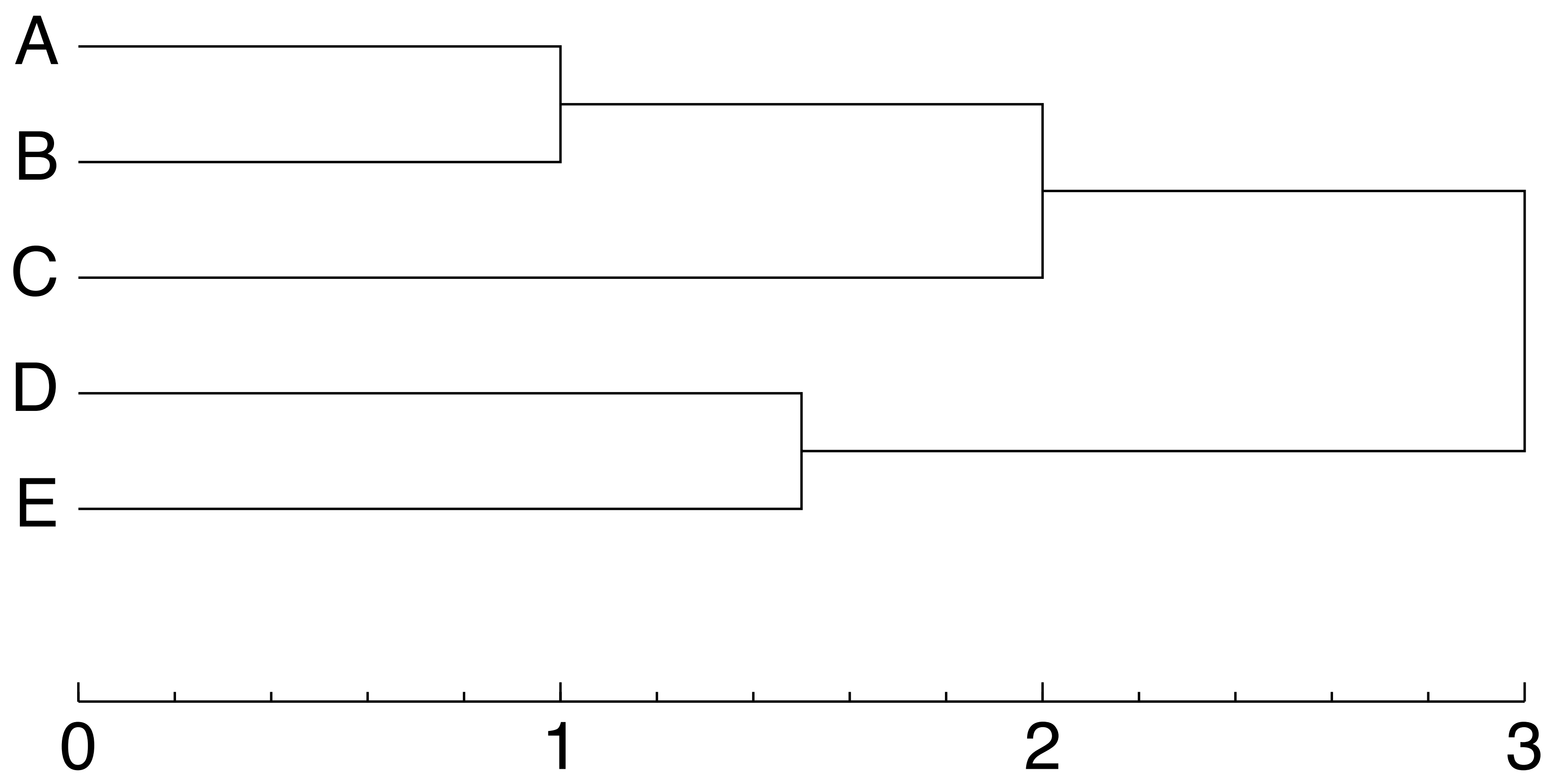
Temporal gene expression data for S. cerevisiae from Kelliher et al. 2016

Clustering methods are algorithms for computing or finding groups in data

Hierarchical Clustering

Clustering Method: Hierarchical Clustering

For n data points define a set of $n - 1$ "joins" that represent the groupings of objects at different levels of similarity. Represent the series of joins as a "tree" graph.



Generic Algorithm for Hierarchical Clustering

1. Calculate a dissimilarity matrix for the n items
2. Join the two nearest items, i and j
3. Delete the i-th and j-th rows and columns of the dissimilarity matrix; and a new row/column that represents the dissimilarity of a new group (i, j) to all other items
4. Repeat from step 2 until there is a single group

Key Point

The different hierarchical clustering methods are determined by the function used to calculate the distance between groups in step 3.

Single Linkage Clustering

Group Distance Measure

Let i and j be groups, and n_i and n_j be the number of objects in the respective groups.

D_{ij} is the *smallest* of the $n_i n_j$ dissimilarities between each element of i and each element of j

Properties of Single Linkage Clustering

- Invariant under monotonic transformation of the d_{ij}
- Unaffected by ties
- Provably nice asymptotic properties
- Disadvantage: susceptible to chaining

More Hierarchical Clustering Functions

Complete Linkage – D_{ij} is the maximum of the $n_i n_j$ dissimilarities between the two groups.

Group Average Methods – D_{ij} is the average of the $n_i n_j$ dissimilarities between the two group (UPGMA, WPGMA)

Centroid Method – D_{ij} is the squared Euclidean distance between the centroids of groups i and j

Hierarchical Clustering, Single Linkage Example

Step 1: Calculate Distance Matrix

Step 2: Find closest elements

	A	B	C	D	E
A	0				
B	4	0			
C	1	4	0		
D	4	2	4	0	
E	5	5	3	4	0

Step 3: Update distance matrix

	(A,C)	B	D	E
(A,C)	0			
B	4	0		
D	4	2	0	
E	3	5	4	0

Worked Example, cont.

Repeat from Step 2

	(A,C)	B	D	E
(A,C)	0			
B	4	0		
D	4	2	0	
E	3	5	4	0

	(A,C)	(B,D)	E
(A,C)	0		
(B,D)	4	0	
E	3	4	0

Repeat from Step 2

	(A,C)	(B,D)	E
(A,C)	0		
(B,D)	4	0	
E	3	4	0

	((A,C),E)	(B,D)
((A,C),E)	0	
(B,D)	4	0

Worked Example, cont.

Repeat from Step 2

	((A,C),E)	(B,D)
((A,C),E)	0	
(B,D)	4	0

Final Join
(((A,C),E),(B,D))

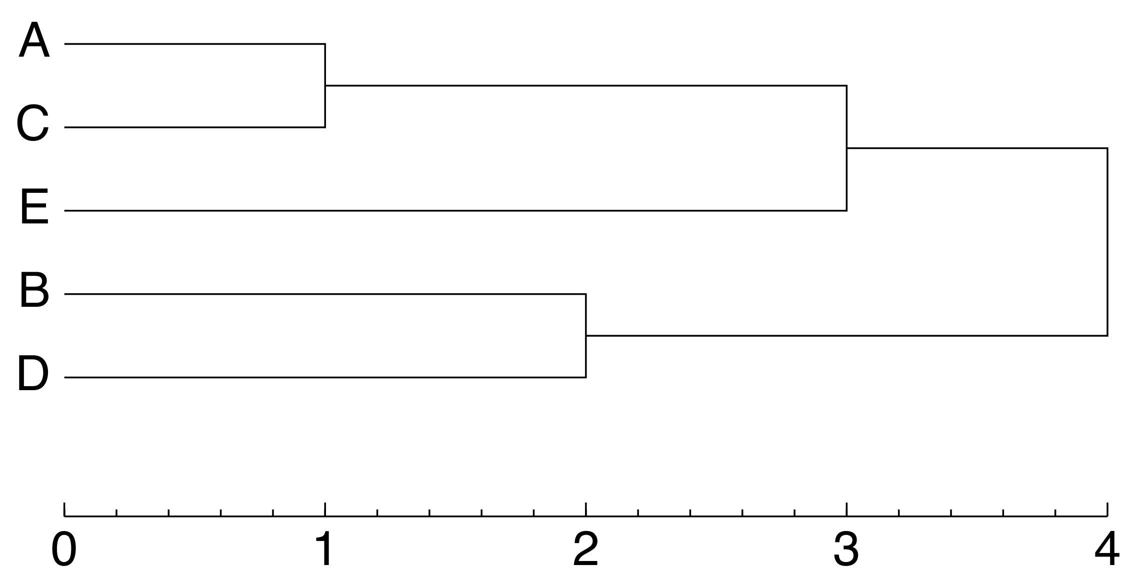


Figure: Final dendrogram for worked example

Dissimilarity Measures for Quantitative Data

This simplest measure of dissimilarity is Euclidean distance.

$$d_{ij} = \left\{ \sum_{k=1}^{p} (x_{ik} - x_{jk})^2 \right\}^{1/2}$$

Dissimilarity Measures for Quantitative Data, cont.

- Manhattan (taxi cab, city block) distance

$$d_{ij} = \sum_{k=1}^{p} |x_{ik} - x_{jk}|$$

- Chebychev distance

$$d_{ij} = max_k \left\{ |x_{ik} - x_{jk}| \right\}$$

- Minkowski Metric

$$d_{ij} = \left\{ \sum_{k=1}^{p} |x_{ik} - x_{jk}|^{\lambda} \right\}^{1/\lambda}$$

$\lambda = 1$ is Manhattan distance, $\lambda = 2$ is Euclidean distance,
$\lambda = \infty$ is Chebychev distance.

Dissimilarity Measures for Variables

Correlation provides a suitable measure of *similarity*. Common *dissimilarity* measures based on correlation include:

- $d_{kl} = 1 - r_{kl}$ if $r_{kl} = -1$ is taken to indicate maximum disagreement
- $d_{kl} = 1 - r_{kl}^2$ if $r_{kl} = 1$ and $r_{kl} = -1$ are treated equivalently (predictive power)
- Based on uncentered correlation:

$$d_{kl} = 1 - \frac{\sum_{i=1}^{n} x_{ik} x_{il}}{\sum_{i=1}^{n} x_{ik}^2 \sum_{i=1}^{n} x_{il}^2}$$

K-means Clustering

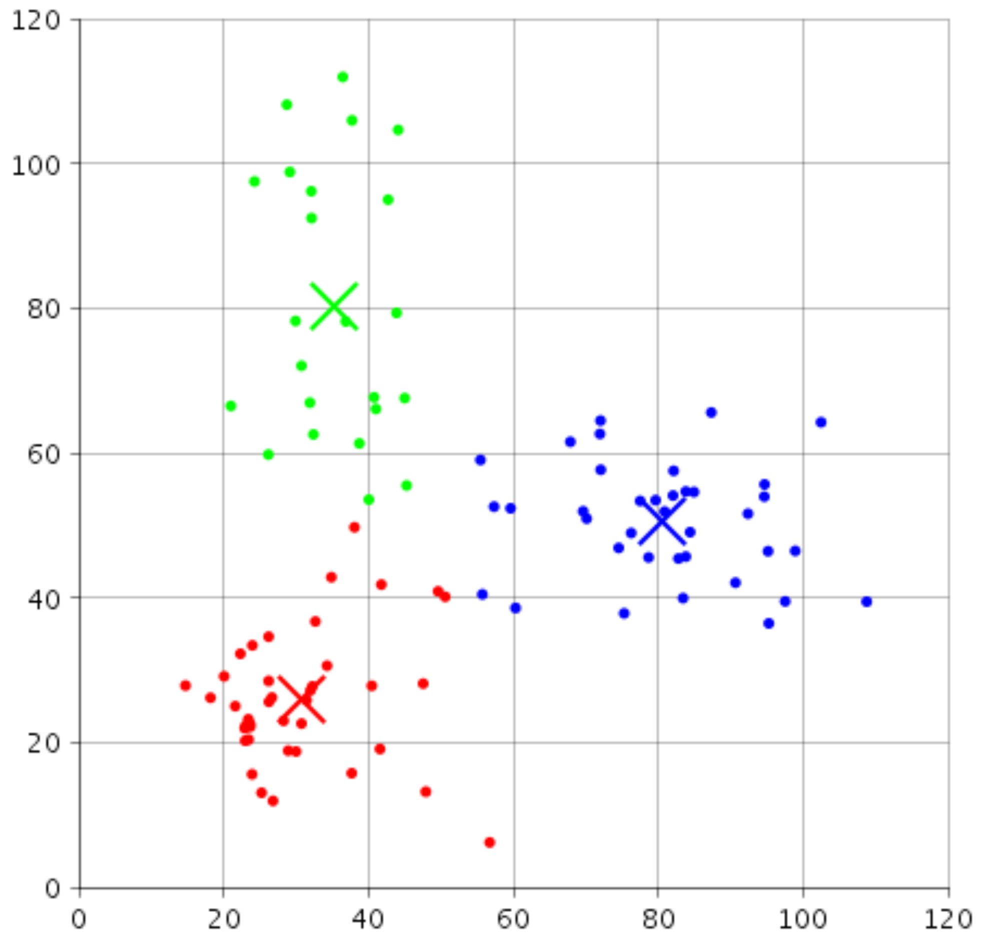
K-mean Clustering

General idea

Assign the n data points (or p variables) to one of K clusters to as to optimize some criterion of interest.

- The most common criterion to minimize is the sum-of-squares from the group centroids.

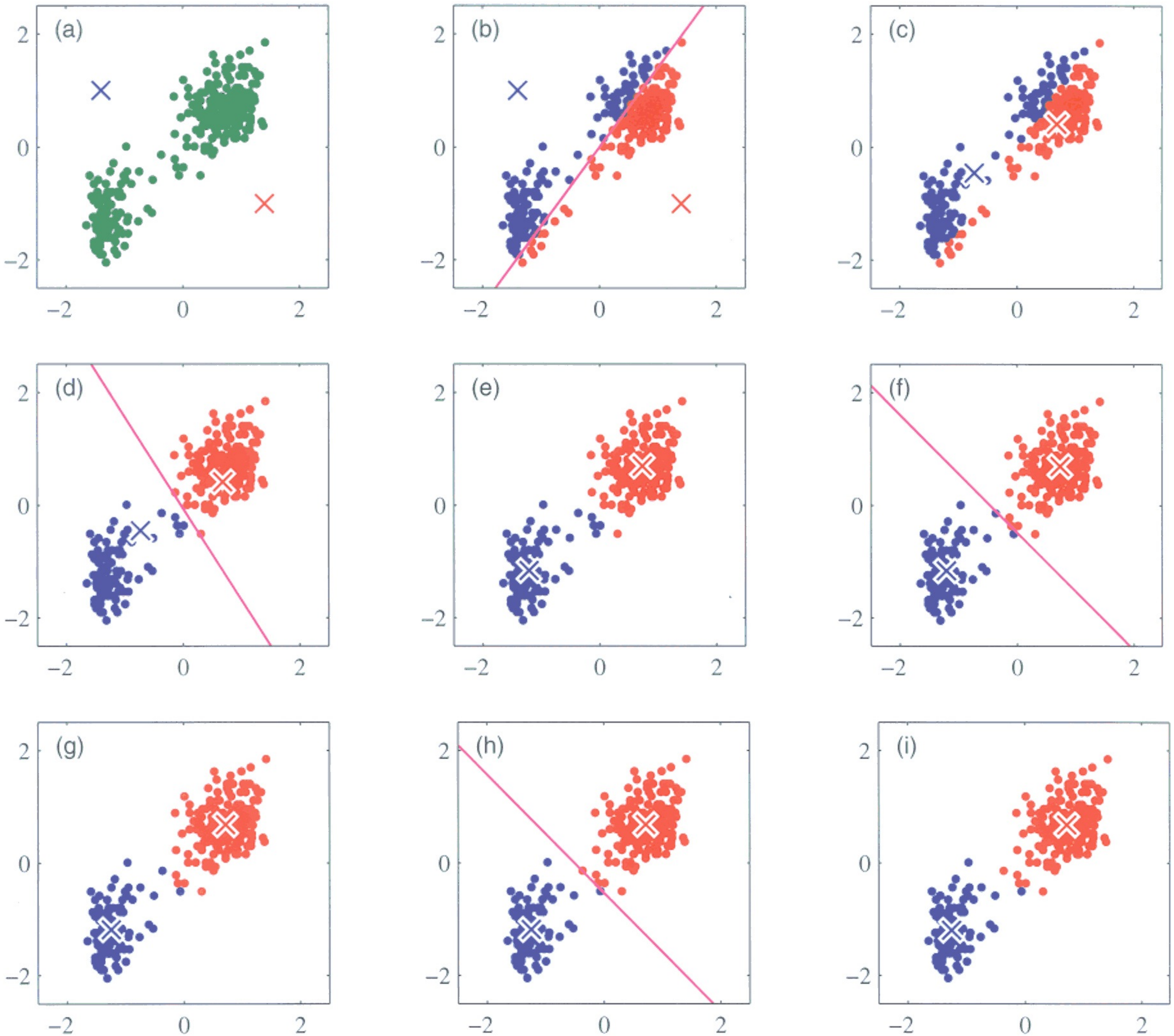
$$V = \sum_{i=1}^{k} \sum_{j \in g_i} |x_j - \mu_i|^2$$



Simple algorithm for K-means clustering

1. Decide on k, the number of groups
2. Randomly pick k of the objects to act as the initial centers
3. Assign each object to the group whose center it is closest to
4. Recalculate the k centers as the centroids of the objects assigned to them
5. Repeat from step 3 until centroids no longer move (convergence)

Illustration of K-means algorithm



Things to note re: K-means clustering

- The algorithm described above does not necessarily find the global optimum

- The algorithm is sensitive to choice of initial cluster center; k-means is often run multiple-time with different initial centers to insure inferred clusters are robust.