COMP5310: Principles of Data Science

W8: Clustering and Dimensionality Reduction

Presented by

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Based on slides by previous lecturers of this unit of study

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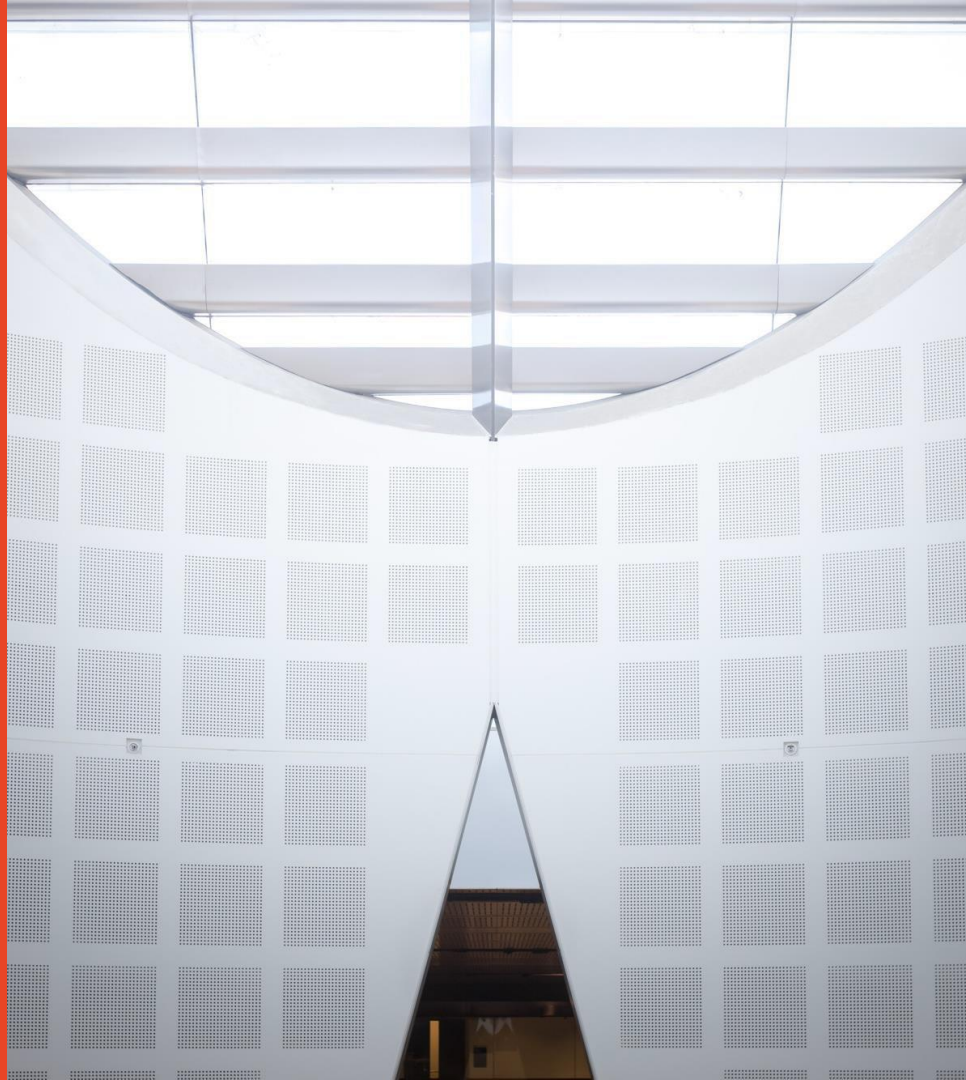


Last week: Association Rule Mining

Objective

Learn techniques for unsupervised learning, with tools in Python.

Lecture

- Association rule mining

Readings

- Intro to Data Mining, Ch. 5
  https://www-users.cse.umn.edu/~kumar001/dmbook/ch5_association_analysis.pdf
- Data Science from Scratch, Ch. 11

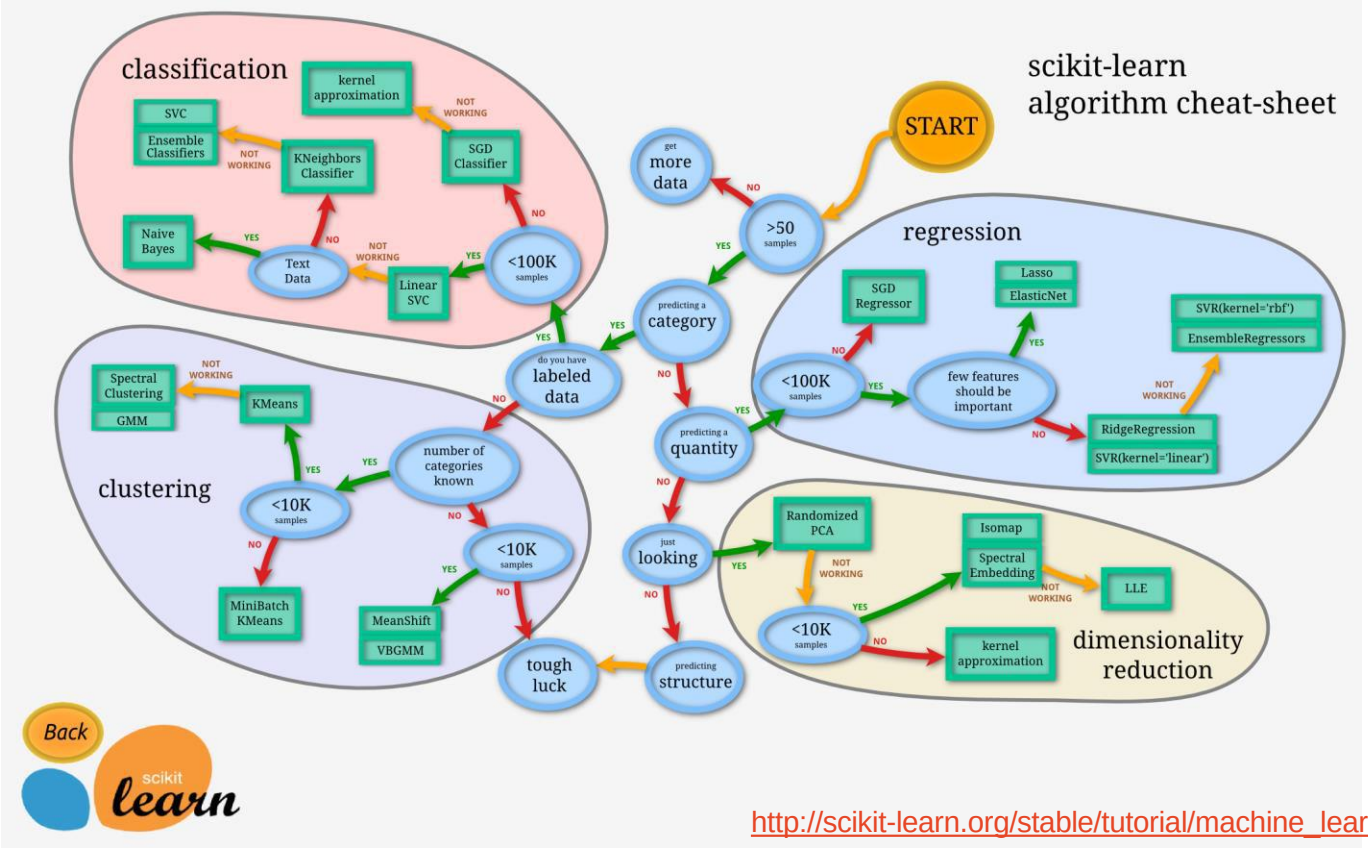
Exercises

- Associations from scratch
- Associations using mlxtend
- Associations using pyfpgrowth

Unsupervised Learning:

- We'll focus on unsupervised machine learning techniques
  - ☑ *Association rule mining*
  - **Clustering**
  - **Dimensionality reduction**
  - Outlier detection
  - Etc.

Machine Learning Map from Scikit-learn



http://scikit-learn.org/stable/tutorial/machine_learning_map/

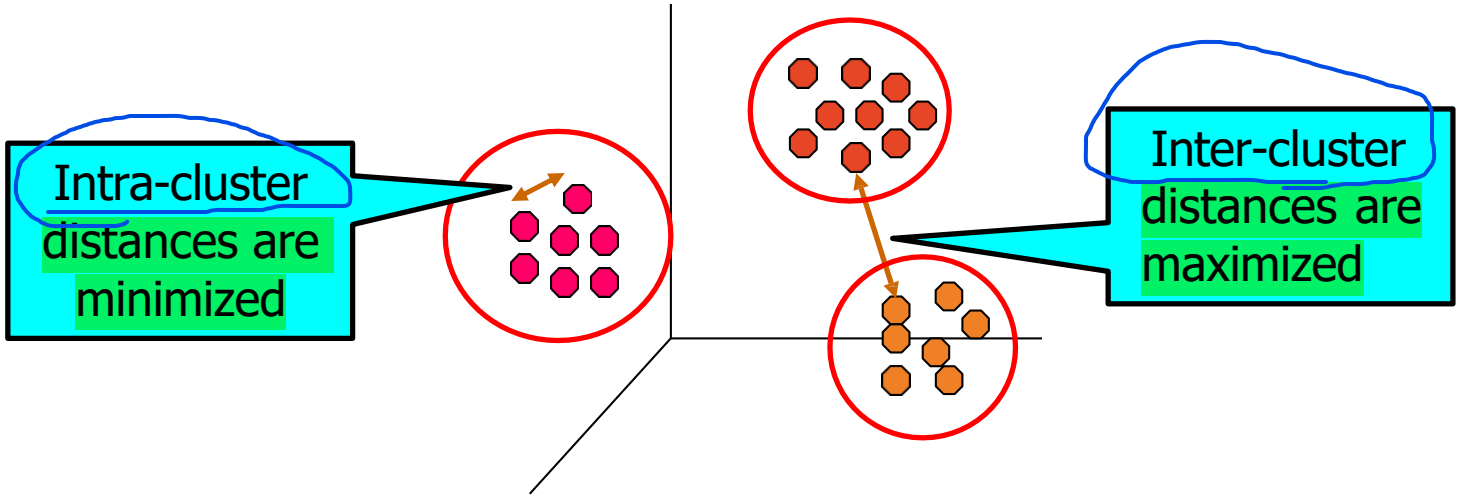
Clustering

Clustering for Understanding

- Group related documents for browsing
- Group genes, proteins, or cells that have similar functionality
- Group stocks with similar price fluctuations
- etc

Clustering: Group Similar Objects

- Group data points into clusters such that
  - Data points in one cluster are more similar to one another.
  - Data points in separate clusters are less similar to one another.
  - Distance function specifies the "closeness" of two objects.



Similarity and Dissimilarity Between Objects

- Distances are normally used to measure the similarity or dissimilarity between two data objects
- Some popular ones include: *Minkowski distance*:

$$d(i,j) = \sqrt[q]{|x_{i1} - x_{j1}|^q + |x_{i2} - x_{j2}|^q + \cdots + |x_{ip} - x_{jp}|^q}$$

where $x_i = (x_{i1}, x_{i2}, \cdots, x_{ip})$ and $x_j = (x_{j1}, x_{j2}, \cdots, x_{jp})$ are two p-dimensional data objects, and q is a positive integer

- If $q = 1$, d is Manhattan distance

$$d(i,j) = |x_{i1} - x_{j1}| + |x_{i2} - x_{j2}| + \cdots + |x_{ip} - x_{jp}|$$

Similarity and Dissimilarity Between Objects (Cont.)

- *If* $q = 2$, d is Euclidean distance: L2 norm

$$d(i,j) = \sqrt{|x_{i1} - x_{j1}|^2 + |x_{i2} - x_{j2}|^2 + \cdots + |x_{ip} - x_{jp}|^2}$$

- Properties
  - $d(i,j) \geq 0$
  - $d(i,i) = 0$
  - $d(i,j) = d(j,i)$
  - $d(i,j) \leq d(i,k) + d(k,j)$

Data Structures

- Data matrix

  n-observations with p-attributes (measurements).

- Dissimilarity matrix $d(i, j)$ is the dissimilarity between objects i and j
  - expresses the pairwise dissimilarities (distances) between observations in the data set
  - the desired data input to some clustering algorithm

attributes/dimensions

tuples/objects

$$\begin{bmatrix} x_{11} & \dots & x_{1f} & \dots & x_{1p} \\ \dots & \dots & \dots & \dots & \dots \\ x & & if & & ip \\ \dots & \dots & \dots & \dots & \dots \\ x_{n1} & \dots & x_{nf} & \dots & x_{np} \end{bmatrix}$$

objects

objects

$$\begin{bmatrix} 0 & & & \\ d(2,1) & 0 & & \\ d(3,1) & d(3, & 0 & \\ : & (& (& \\ ,2) & \dots \dots & & 0 \end{bmatrix}$$

Types of Clusterings

Important distinction between hierarchical and partitional sets of clusters

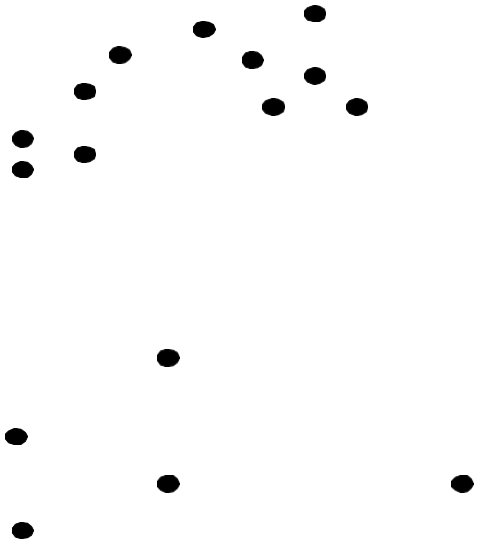
- ***Partitional clustering***

  A division of data objects into non-overlapping subsets (clusters) such that each data object is in exactly one subset

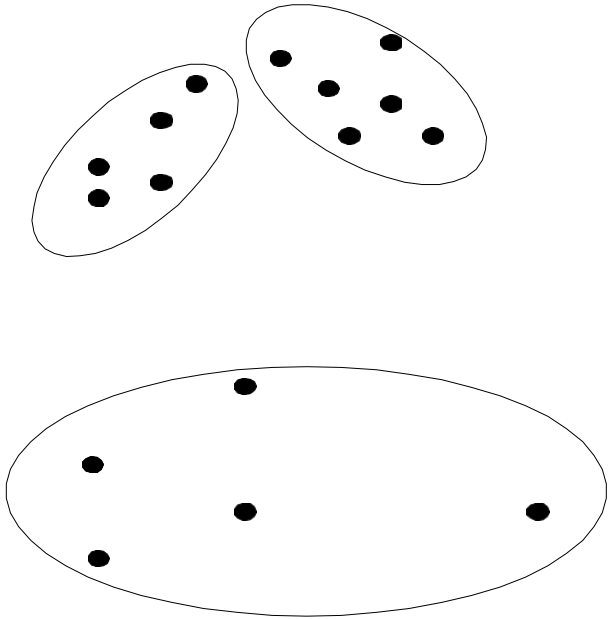
- ***Hierarchical clustering***

  A method of cluster analysis which seeks to build a hierarchy of clusters. It produces a set of nested clusters organized as a hierarchical tree

Partitional Clustering



Original Points



A Partitional Clustering

Partitional Clustering: K-Means Clustering

- Number of clusters, *k*, must be specified
- Each cluster is associated with a centroid (center point)
- Each point is assigned to the cluster with the closest centroid
- The basic algorithm is very simple

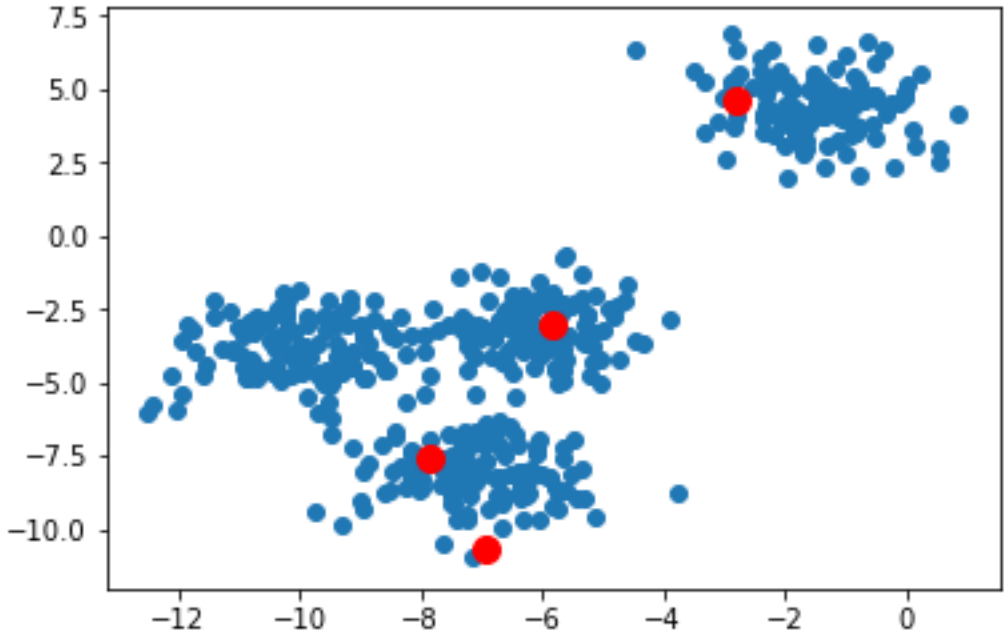
1: Select K points as the initial centroids.
2: **repeat**
3: Form K clusters by assigning all points to the closest centroid.
4: Recompute the centroid of each cluster.
5: **until** The centroids don't change

K-Means Clustering – Details

- Initial centroids are often chosen randomly
- Clusters produced vary from one run to another
- K-means will converge for common similarity measures
- Most of the convergence happens in the first few iterations
- Complexity is $O(n \times k \times i \times d)$
  - n = number of points, k = number of clusters, i = number of iterations, d = number of attributes (or dimensions)

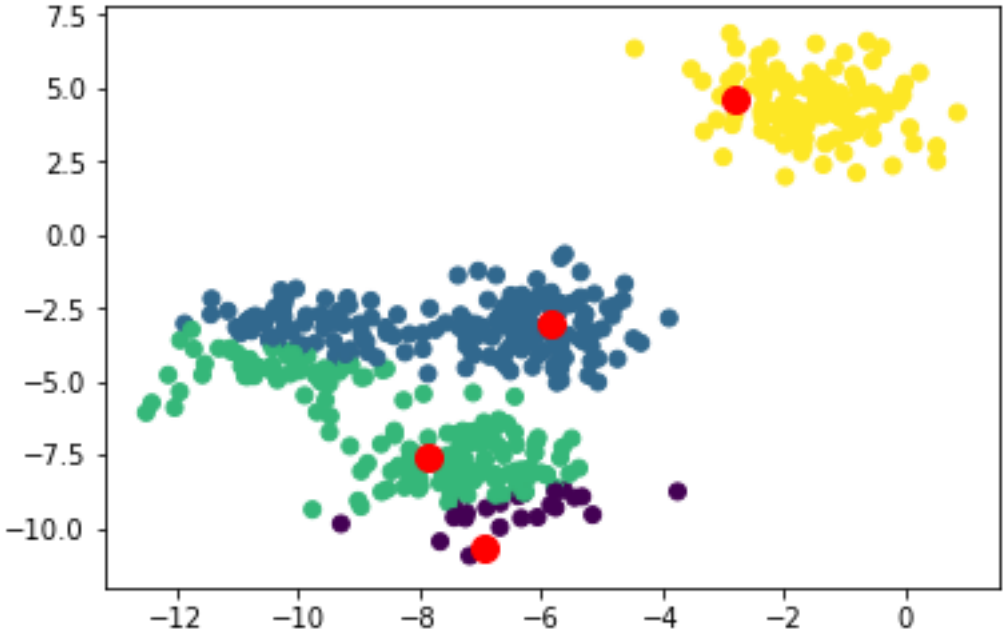
K-Means Example

- Number of clusters: K = 4
- Initialize 4 centroids randomly



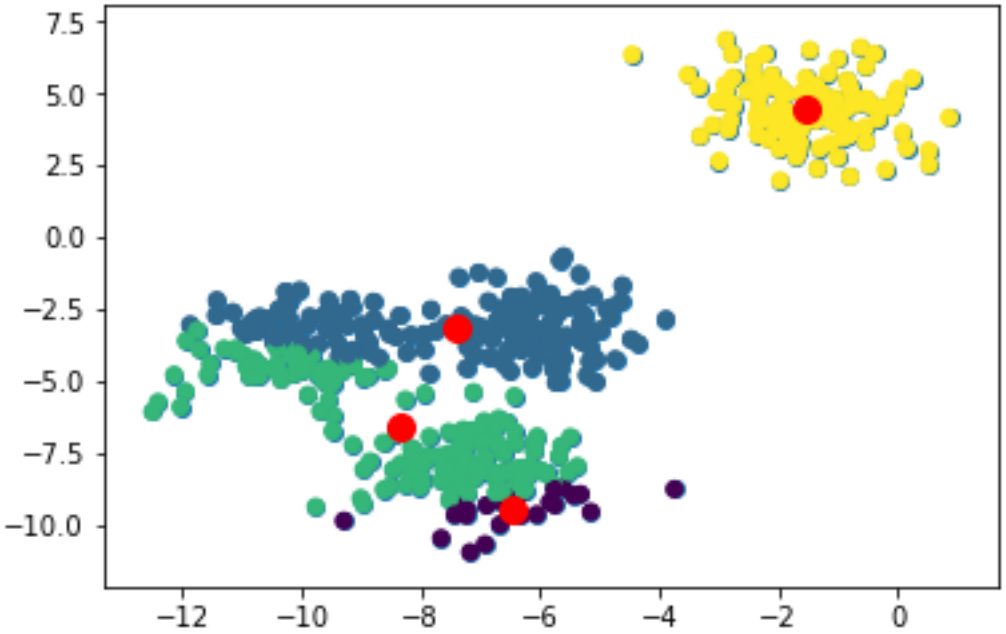
K-Means Example (Cont.)

– Assigned each point to the cluster with the closest centroid



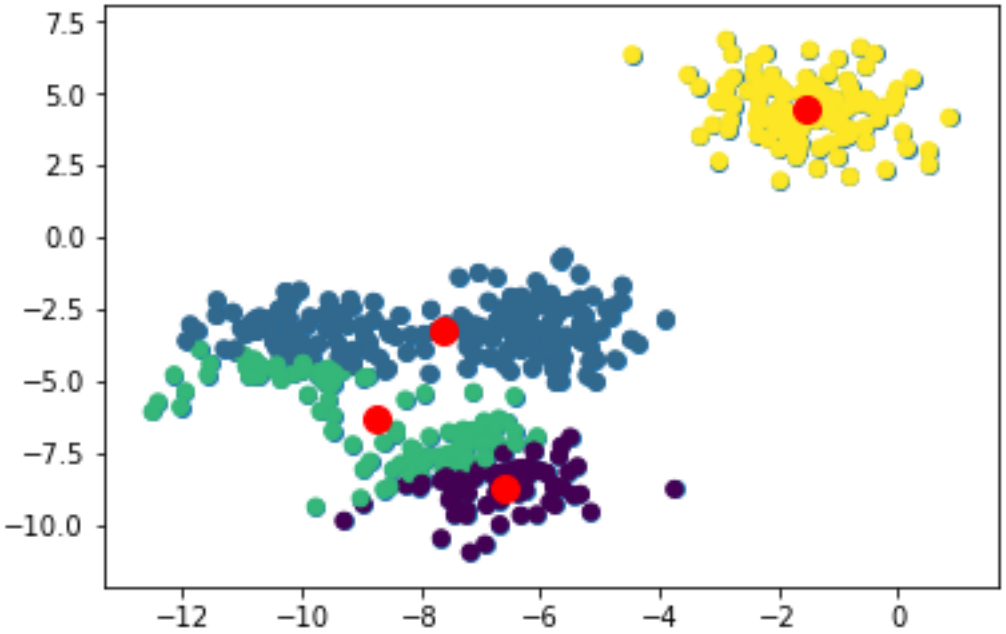
K-Means Example (Cont.)

– Re-compute each cluster center to be the mean of the points previously assigned.



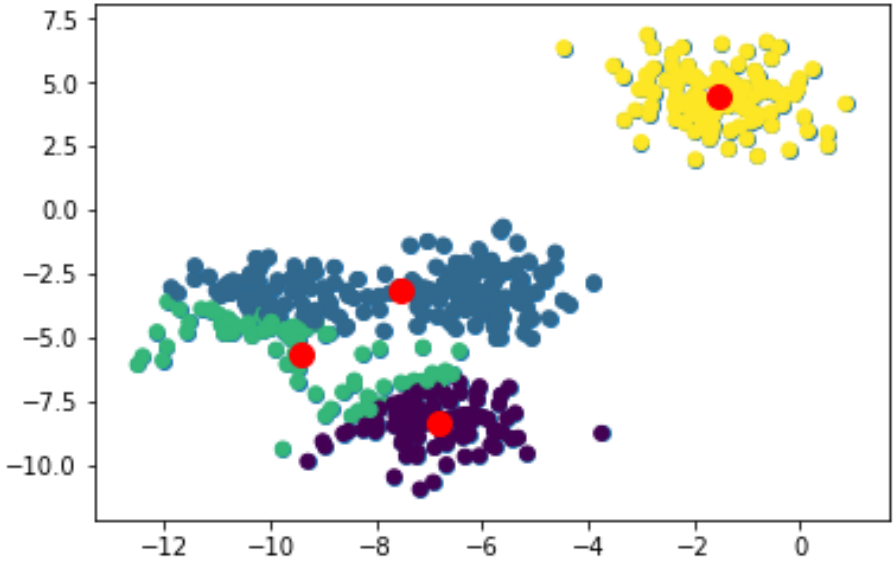
K-Means Example (Cont.)

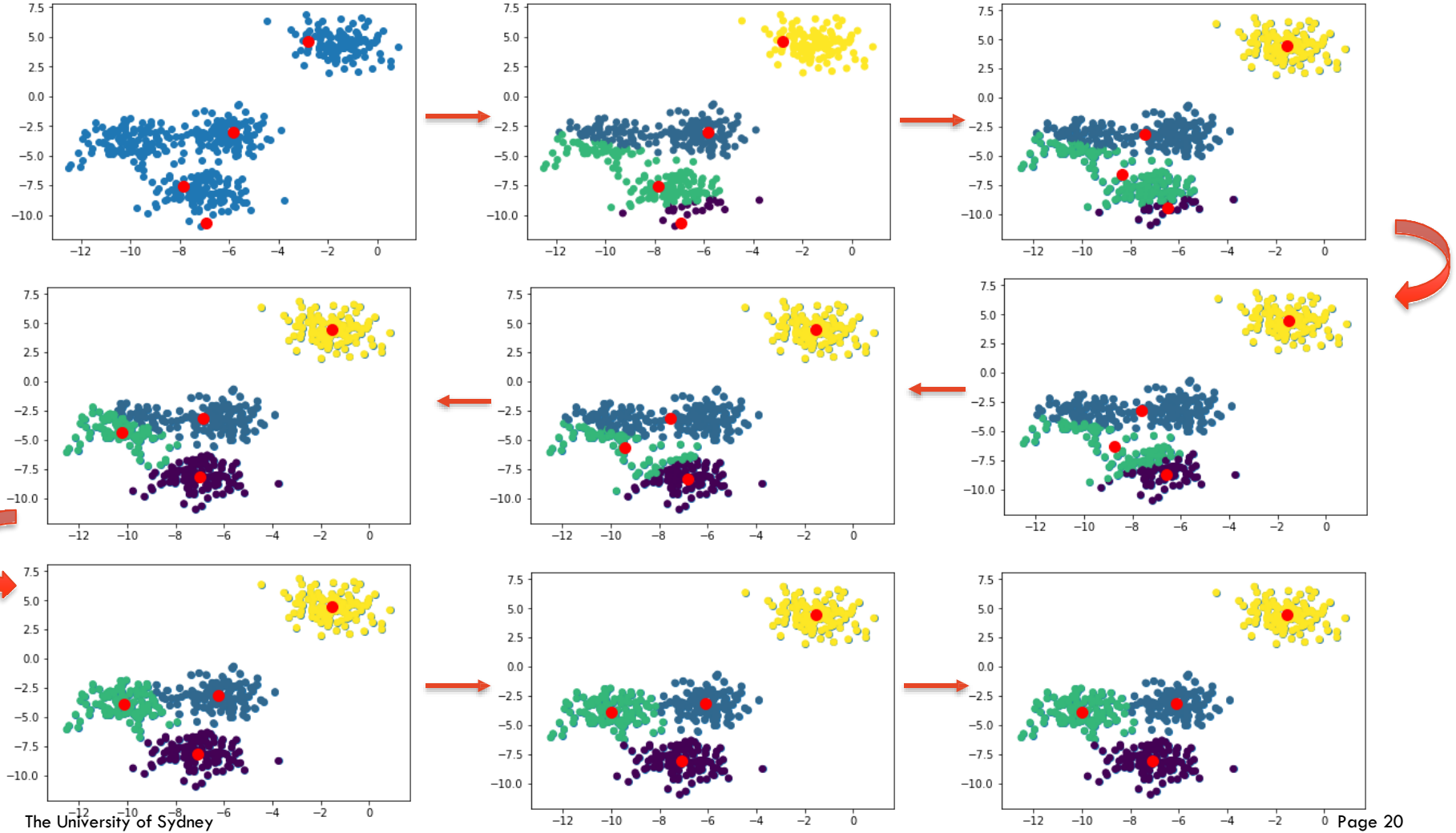
– Assigned each point to the cluster with the closest centroid



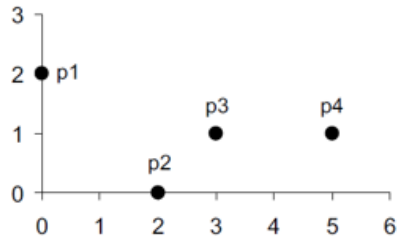
K-Means Example (Cont.)

- Re-compute each cluster center
- Centroid changed?
  - Assigned each point to the cluster with the closest centroid
  - Re-compute each cluster center





point	x	y
p1	0	2
p2	2	0
p3	3	1
p4	5	1



Pairwise Euclidean Distances:

1. p1-p2
   $\sqrt{(2-0)^2 + (0-2)^2} = \sqrt{4+4} = \sqrt{8} \approx 2.83$

2. p1-p3
   $\sqrt{(3-0)^2 + (1-2)^2} = \sqrt{9+1} = \sqrt{10} \approx 3.16$

3. p1-p4
   $\sqrt{(5-0)^2 + (1-2)^2} = \sqrt{25+1} = \sqrt{26} \approx 5.10$

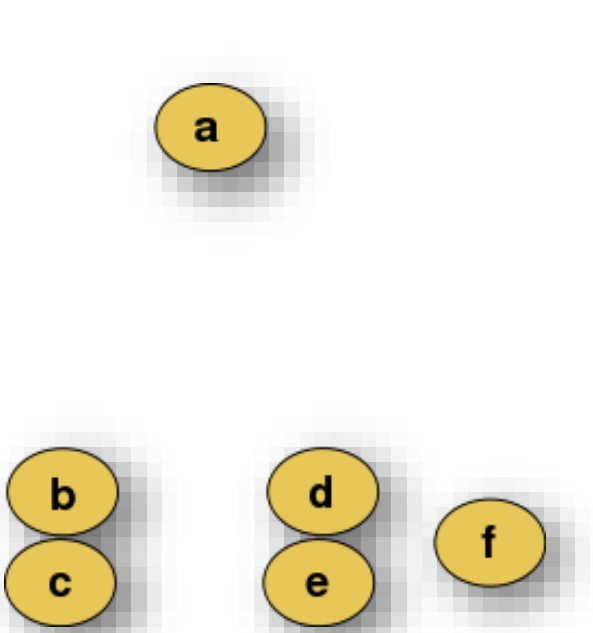
4. p2-p3
   $\sqrt{(3-2)^2 + (1-0)^2} = \sqrt{1+1} = \sqrt{2} \approx 1.41$

5. p2-p4
   $\sqrt{(5-2)^2 + (1-0)^2} = \sqrt{9+1} = \sqrt{10} \approx 3.16$

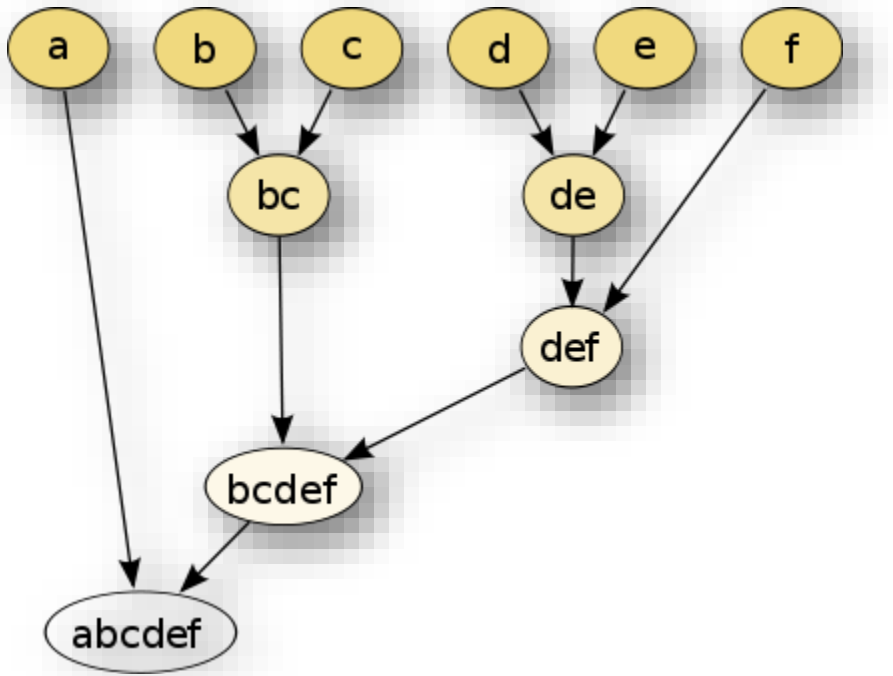
6. p3-p4
   $\sqrt{(5-3)^2 + (1-1)^2} = \sqrt{4+0} = \sqrt{4} = 2.00$

L2	p1	p2	p3	p4
p1	0	2.828	3.162	5.099
p2	2.828	0	1.414	3.162
p3	3.162	1.414	0	2
p4	5.099	3.162	2	0

Hierarchical Clustering



Original Data Items



Hierarchical Clustering

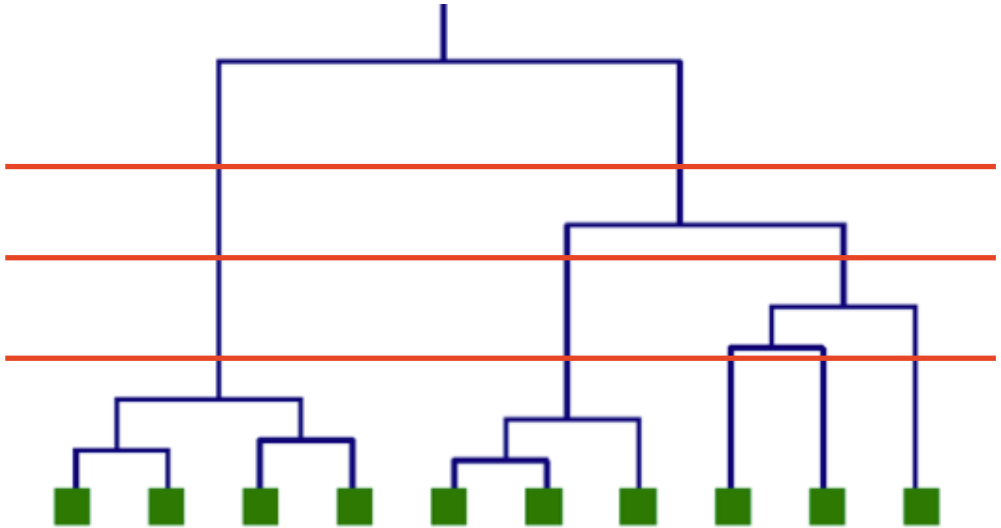
Hierarchical Clustering

Strategies for hierarchical clustering generally fall into two types:

- **Agglomerative**: This is a "bottom up" approach: each object starts in its own cluster, and pairs of clusters are merged as one moves up the hierarchy.
- **Divisive**: This is a "top down" approach: all objects start in the same cluster, and splits are performed recursively as one moves down the hierarchy.

Hierarchical Clustering: e.g. Agglomerative

- Initial
  - Each point in its own cluster
- Repeat
  - Find closest pair of clusters
    - Min-distance between any two points
  - Merge them into one cluster
  - Recompute distances between new cluster and others
- Until
  - Desired number of clusters remaining e.g. single cluster

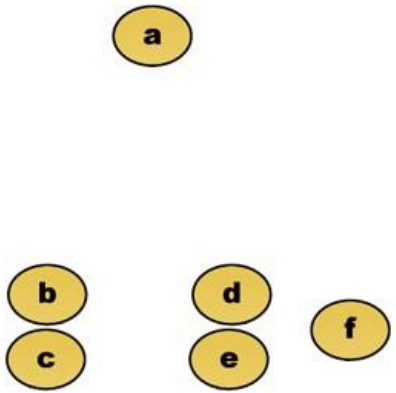


dendrogram

Hierarchical Algorithm

Steps in Hierarchical Algorithm:

- The first step generates the distance calculation matrix for each data item as shown in table below, in this case: {a}, {b}, {c}, {d}, {e}, {f}.



	a	b	c	d	e	f
a	0	184	222	177	216	231
b	184	0	45	123	128	200
c	222	45	0	129	121	203
d	177	123	129	0	46	83
e	216	128	121	46	0	83
f	231	200	203	83	83	0

Hierarchical Algorithm

- Next step is to merge the closest data items.
  - In this case: {b , c} are merged.
  - Therefore, the first clustering process generates: {a}, {b, c}, {d},{e},{f}.

	a	b	c	d	e	f
a	0	184	222	177	216	231
b	184	0	45	123	128	200
c	222	45	0	129	121	203
d	177	123	129	0	46	83
e	216	128	121	46	0	83
f	231	200	203	83	83	0

	a	b,c	d	e	f
a	0	?	177	216	231
b,c	?	0	?	?	?
d	177	?	0	46	83
e	216	?	46	0	83
f	231	?	83	83	0

Hierarchical Algorithm

Distance Calculation between two clusters:

- single linkage:
  - The minimum distance between elements of the two clusters
- complete linkage:
  - The maximum distance between elements of the two clusters
- average linkage: i.e. mean distance calculation.

Hierarchical Algorithm with Single Linkage

- Repeat the distance calculation process based on single linkage
- Apply merging process based on previous merged results.
  - In this case: {d, e} are merged.
- The final results are: {a}, {b, c} {d, e} {f} → {a}, {b, c}, {d, e, f} → {a}, {b, c, d, e, f} → {a, b, c, d, e, f}

	a	b	c	d	e	f
a	0	184	222	177	216	231
b	184	0	45	123	128	200
c	222	45	0	129	121	203
d	177	123	129	0	46	83
e	216	128	121	46	0	83
f	231	200	203	83	83	0

	a	b, c	d	e	f
a	0	184	177	216	231
b, c	184	0	123	121	200
d	177	123	0	46	83
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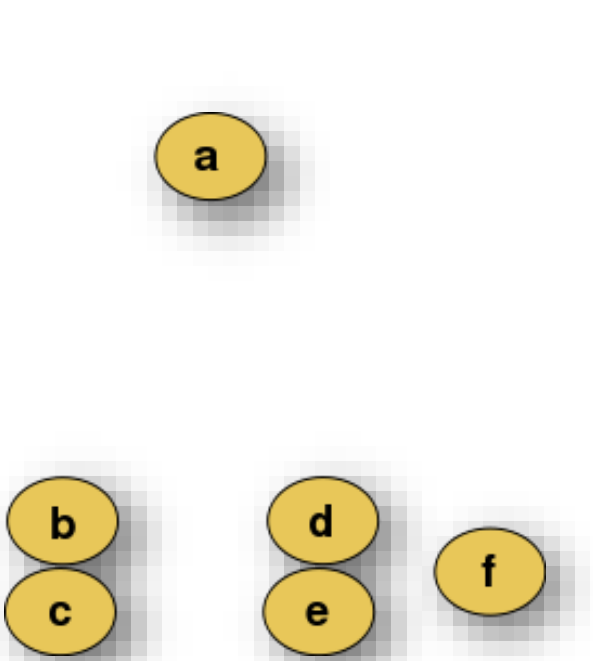
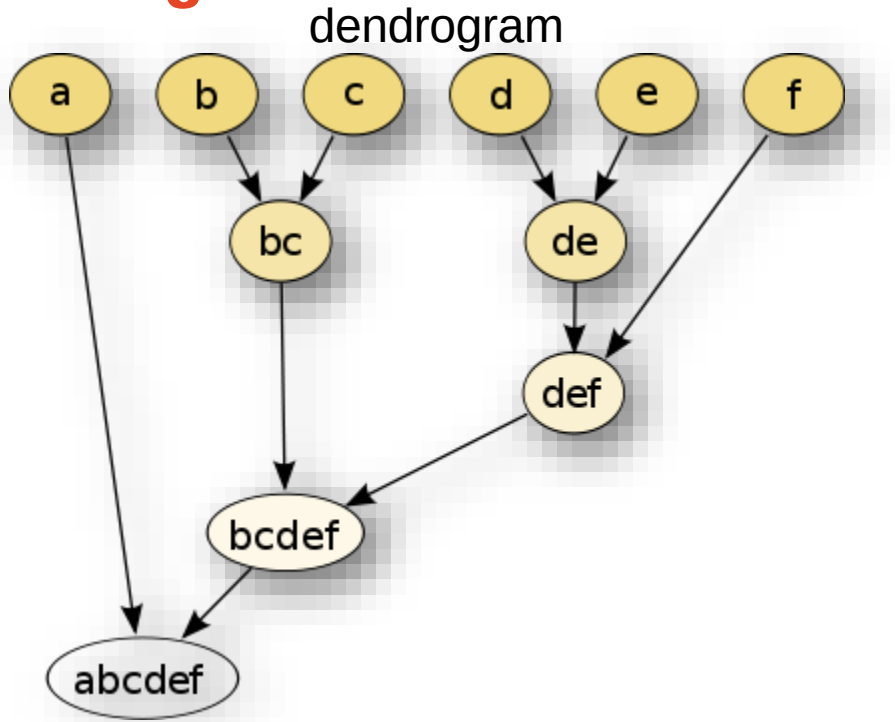
f	231	200	83	83	0

Resultant Hierarchical Clustering



Original Data Items



Hierarchical Clustering

Evaluating Clustering

Cluster Validity

- For supervised classification, we have a variety of measures to evaluate how good our model is (accuracy, precision, recall) –
- For cluster analysis, the analogous question is how to evaluate the "goodness" of the resulting clusters.
- While clusters are in the eye of the beholder, we may still want to evaluate them…
  - To avoid finding patterns in noise
  - To compare clustering algorithms
  - To compare two sets of clusters
- https://scikit-learn.org/stable/modules/clustering.html#clustering-performance-evaluation

Measures of Cluster Validity

Numerical measures that are applied to judge various aspects of cluster validity, are classified into the following three types.

- External Index: Measure the extent to which cluster labels match externally supplied class labels (e.g., accuracy, precision, recall, F1-score)
- Internal Index: Measure the goodness of a clustering structure *without* respect to external information (e.g., Sum of Squared Error)
- Relative Index: Compare two different clusterings or clusters (often an external or internal index is used)

External Evaluation Measures

- Homogeneity ranges from 0 to 1, preferring each cluster contains only members of a single class.
  (analogous to precision, $P = TP / (TP+FP)$)
- Completeness ranges from 0 to 1, preferring all members of a given class are assigned to the same cluster
  (analogous to recall, $R = TP / (TP+FN)$)
- V-measure is the harmonic mean of homogeneity and completeness
  (analogous to F1 score = 2PR / (P+R))
- http://scikit-learn.org/stable/modules/clustering.html#homogeneity-completeness-and-v-measure

Internal: Sum of Squared Error (SSE)

- For each point, the error is the distance to the nearest cluster
- To get SSE, we square these errors and sum them.

$$SSE = \sum_{i=1}^{K} \sum_{x \in C_i} dist^2(x, m_i)$$

- x is a data point in cluster C_i and m_i is the centroid point (mean) for cluster C_i

SSE Example

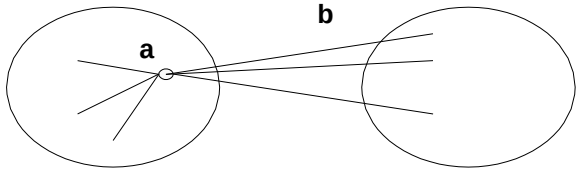
- Suppose we have 3 clusters:
  - Cluster 1: [2, 4] with centroid at 3
  - Cluster 2: [5, 6, 7] with centroid at 6
  - Cluster 3: [8, 10, 12] with centroid at 10
- Squared error for each cluster:
  - $SE1 = (2-3)^2 + (4-3)^2 = 1 + 1 = 2$
  - $SE2 = (5-6)^2 + (7-6)^2 = 1 + 1 = 2$
  - $SE3 = (8-10)^2 + (12-10)^2 = 4 + 4 = 8$
- $SSE = SE1 + SE2 + SE3 = 12$

Internal: Silhouette Coefficient

- For an individual point *x*
  - Calculate ***a*** = average distance of *x* to points in its cluster
  - Calculate ***b*** = average distance of *x* to points in the next nearest cluster
  - The silhouette coefficient for a point is then given by

    $s = 1 - a/b$ if $a < b$, (or $s = b/a - 1$ if $a \geq b$, not the usual case)

  - The closer to 1 the better



- Silhouette coefficient for dataset is average across all *data points*

Silhouette Coefficient Example

- Suppose we have 3 clusters:
  - Cluster 1 = [[1,0], [1,1]]
  - Cluster 2 = [[1,2], [2,3], [2,2], [1,2]],
  - Cluster 3 = [[3,1], [3,3], [2,1]]
- Take a point [1,0] in cluster 1
- Calculate its average distance to all other points in its cluster, i.e. cluster 1
- So a1 = $\sqrt{(1-1)^2 + (0-1)^2} = \sqrt{0+1} = 1$

Silhouette Coefficient Example (Cont.)

- Now for the point [1,0] in cluster 1 calculate its average distance from all the points in cluster 2 and cluster 3.
- Of these take the minimum average distance.
- So for cluster 2:
  - [1,0] → [1,2], distance = $\sqrt{(1-1)^2 + (0-2)^2} = \sqrt{0+4} = 2$
  - [1,0] → [2,3], distance = $\sqrt{(1-2)^2 + (0-3)^2} = \sqrt{1+9} = 3.16$
  - [1,0] → [2,2], distance = $\sqrt{(1-2)^2 + (0-2)^2} = \sqrt{1+4} = 2.24$
  - [1,0] → [1,2], distance = $\sqrt{(1-1)^2 + (0-2)^2} = \sqrt{0+4} = 2$
- Therefore, the average distance of point [1,0] in cluster 1 to all the points in cluster 2 = $(2+3.16+2.24+2)/4 = 2.35$

Silhouette Coefficient Example (Cont.)

- Similarly, for cluster 3.
  - [1,0] → [3,1], distance = $\sqrt{(1-3)^2 + (0-1)^2} = \sqrt{4+1} = 2.24$
  - [1,0] → [3,3], distance = $\sqrt{(1-3)^2 + (0-3)^2} = \sqrt{4+9} = 3.61$
  - [1,0] → [2,1], distance = $\sqrt{(1-2)^2 + (0-1)^2} = \sqrt{1+1} = 1.41$
- Therefore, the average distance of point [1,0] in cluster 1 to all the points in cluster 3 = (2.24+3.61+1.41)/3 = 2.42
- Now, the minimum average distance of the point [1,0] in cluster 1 to the other clusters 2 and 3 is,

  b1 =2.35 (2.35 < 2.42)

Silhouette Coefficient Example (Cont.)

- So the silhouette coefficient of point [1,0] in cluster 1

$$s1 = 1-(a1/b1) = 1- (1/2.35) = 1-0.43 = 0.57$$

- In a similar fashion you need to calculate the silhouette coefficient for each data point in each cluster
- Then we average them to calculate the overall silhouette coefficient to evaluate the resultant clusters
- The closer to 1 the better

Choosing *k*

Notion of a Cluster can be Ambiguous

How many clusters..?

Maybe six clusters

Two clusters?

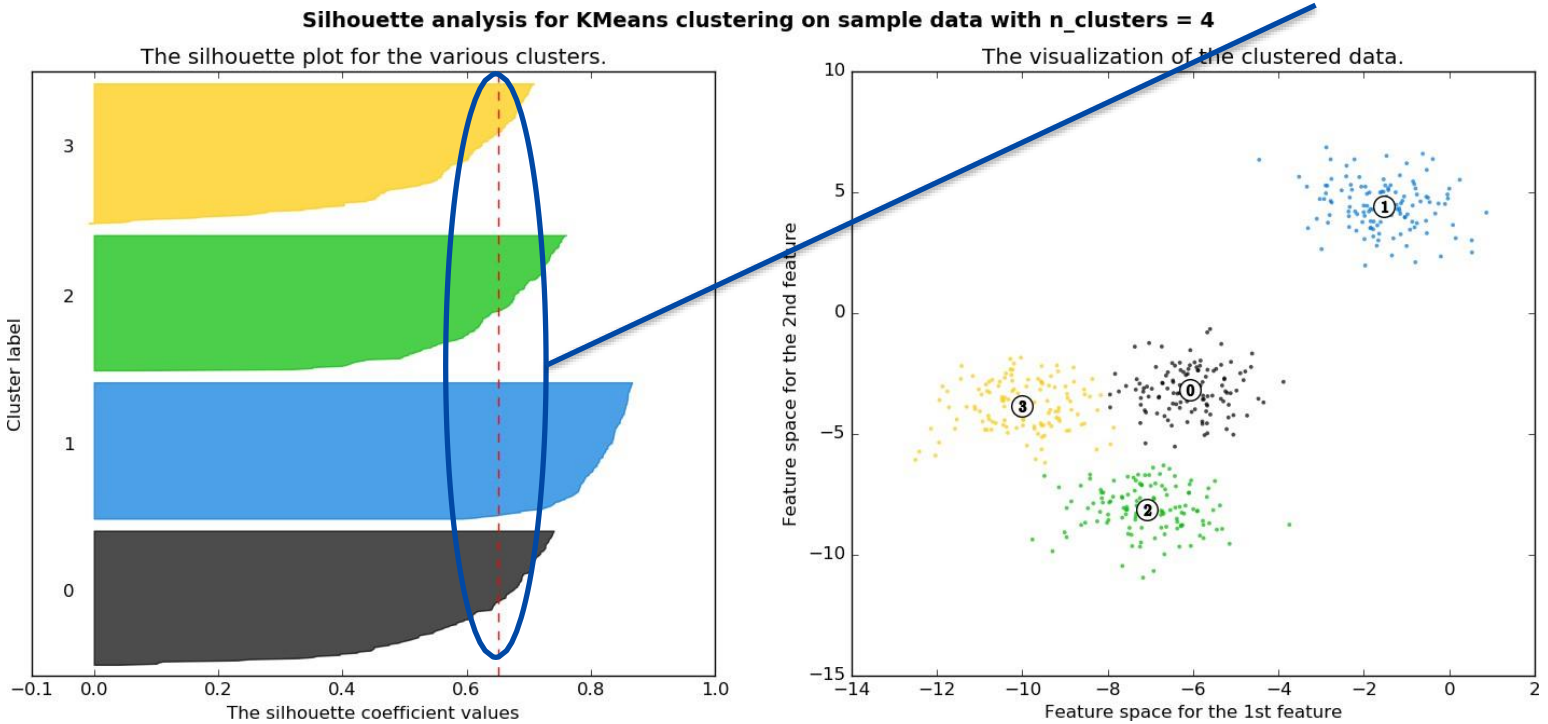
Or four clusters

Choosing *k*

- Often we don't know the number of clusters in our data
- Selecting *k* is generally an interactive process
- There are some approaches to aid interactive selection, and sometimes automate it

Using Silhouettes to choose *k*

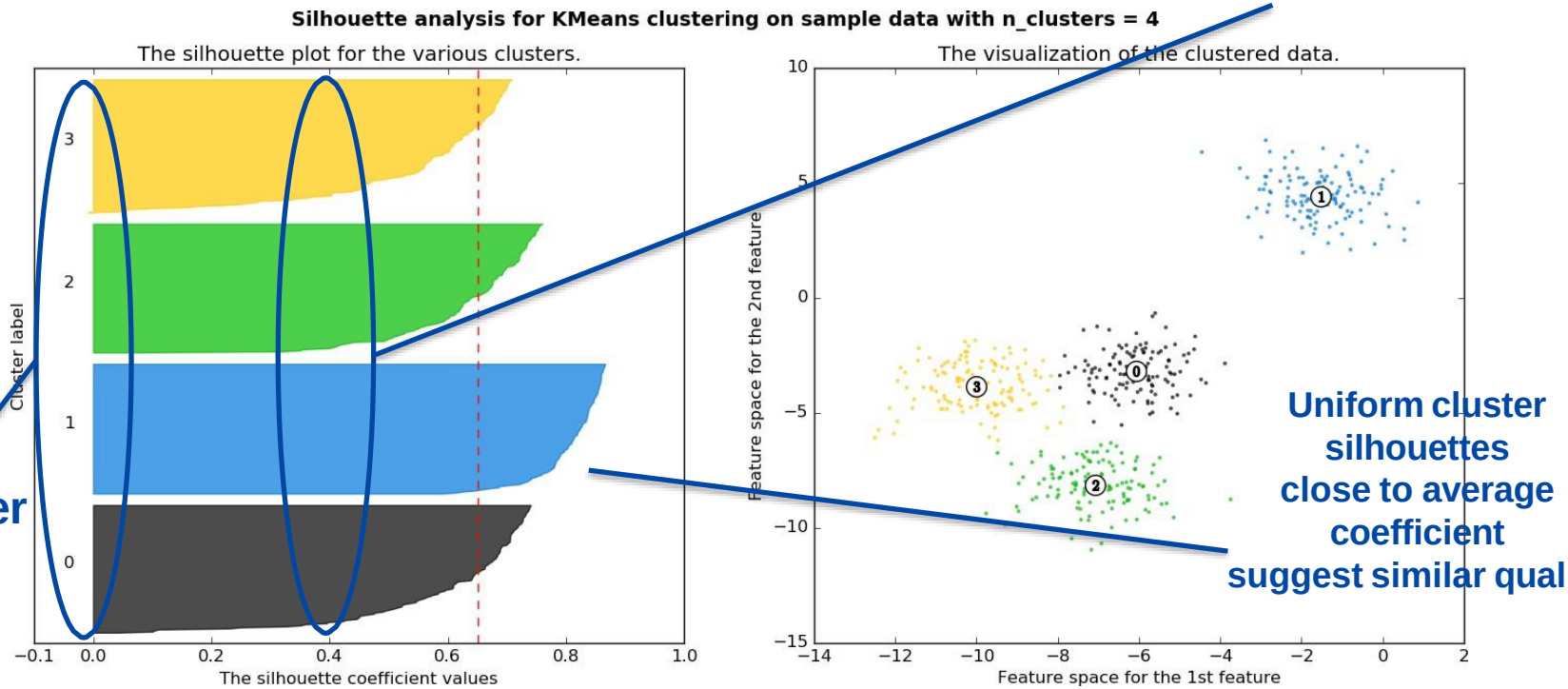
High average silhouette indicates points far away from neighbouring clusters



http://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_silhouette_analysis.html

Using Silhouettes to choose *k*

Bar chart showing silhouette values for each item grouped by cluster



Cluster IDs

Uniform cluster silhouettes close to average coefficient suggest similar quality

http://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_silhouette_analysis.html

Pre-Processing for Clustering

We only looked at choosing *k*, but more pre-processing needed

- Data Cleansing
- Data Transformation
- **Data Normalisation**
- **Dimensionality Reduction** / choice or projection of dimensions
  - closely related to choice of **distance metric**
  - we used Euclidean Metric so far (L_2-Norm)
  - but others possible too, eg. Manhatten Distance (L_1-Norm)
  - "Curse of high dimensionality"; cf Aggarwal et al.: "On the Surprising Behavior of Distance Metrics in High Dimensional Space", 2001.

Principal Component Analysis

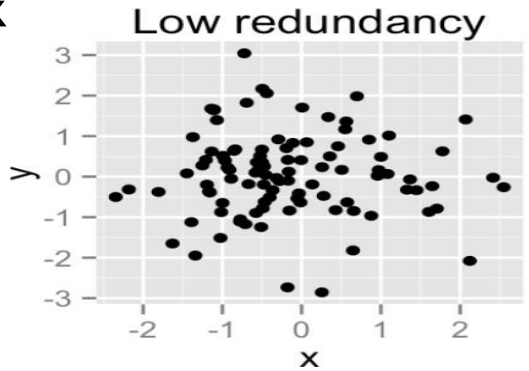
Principal Components Analysis

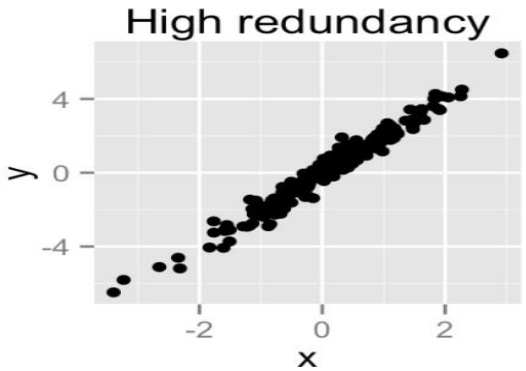
- Aims to transform the original data from high dimensional space into lower dimensional space.
- The new variables in the lower dimensional space corresponds to a linear combination of the originals and are called principal components (PC)
- PCA helps in
  - **Visualization**. Using the right variables to plot items will give more insights.
  - **Uncovering Clusters**. With good visualizations, hidden categories or clusters could be identified.
  - **Dimensionality reduction.** Reduce number of dimensions in data

Principal Components Analysis

- PCA method is particularly useful when the variables within the data set are highly correlated.
  - Correlation indicates that there is redundancy in the data.
  - Correlation is captured by the covariance matrix[1].
- PCA is traditionally performed on covariance matrix or correlation matrix

[1]covariance matrix is a square **matrix** that contains the variances and **covariances** associated with several variables.





Covariance Matrix

- Representing Covariance between dimensions as a matrix e.g for three attributes (x,y,z):

$$C = \begin{pmatrix} \mathrm{cov}(x,x) & \mathrm{cov}(x,y) & \mathrm{cov}(\\ \mathrm{cov}(y,x) & \mathrm{cov}(y,y) & \mathrm{cov}(\\ \mathrm{cov}(z,x) & \mathrm{cov}(z,y) & \mathrm{cov}(\end{pmatrix}$$

Variances

- The covariance between one dimension and itself is the variance
  - Diagonal is the variances of x, y and z
- cov(x,y) = cov(y,x) hence matrix is symmetrical about the diagonal
- N-dimensional data will result in NxN covariance matrix

Covariance Matrix Example

- Below is the covariance matrix of some 3 variables.
- Their variances are on the diagonal, and the sum of the 3 values (3.448) is the overall variability

1.343730	-.1601522	.1864702
-.1601522	.61920562	-.1266842
.1864702	-.1266842	1.485549

- In the covariance table above, the off-diagonal values are different from zero. This indicates the presence of redundancy in the data.
- In other words, there is a certain amount of correlation between variables.

PCA Example

- PCA creates uncorrelated PC variables (called eigenvectors) having zero covariations and variances (called eigenvalues) sorted in decreasing order.
- The first PC captures the greatest variance, the second greatest variance is the second PC, and so on.
- By eliminating the later PCs we can achieve dimensionality reduction.
  - The 1st PC accounts for or "explains" 1.651/3.448 = 47.9% of the overall variability;
  - the 2nd one explains 35.4% of it; the 3rd one explains 16.7% of it.

1.65135	.000000	.000000
.000000	1.220288	.000000
.000000	.0000000	.576843

The covariance matrix between the principal components

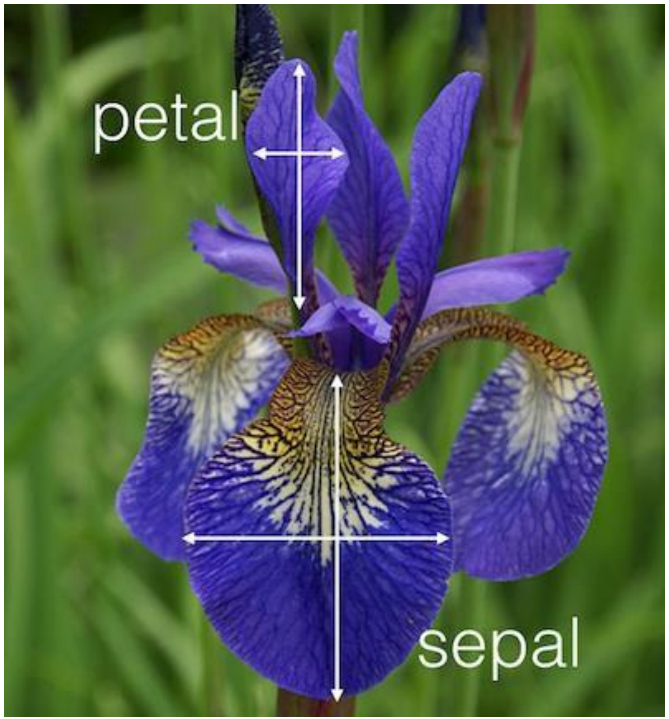
PCA on Iris Dataset

- Iris data has 150 observations equally distributed among three species:

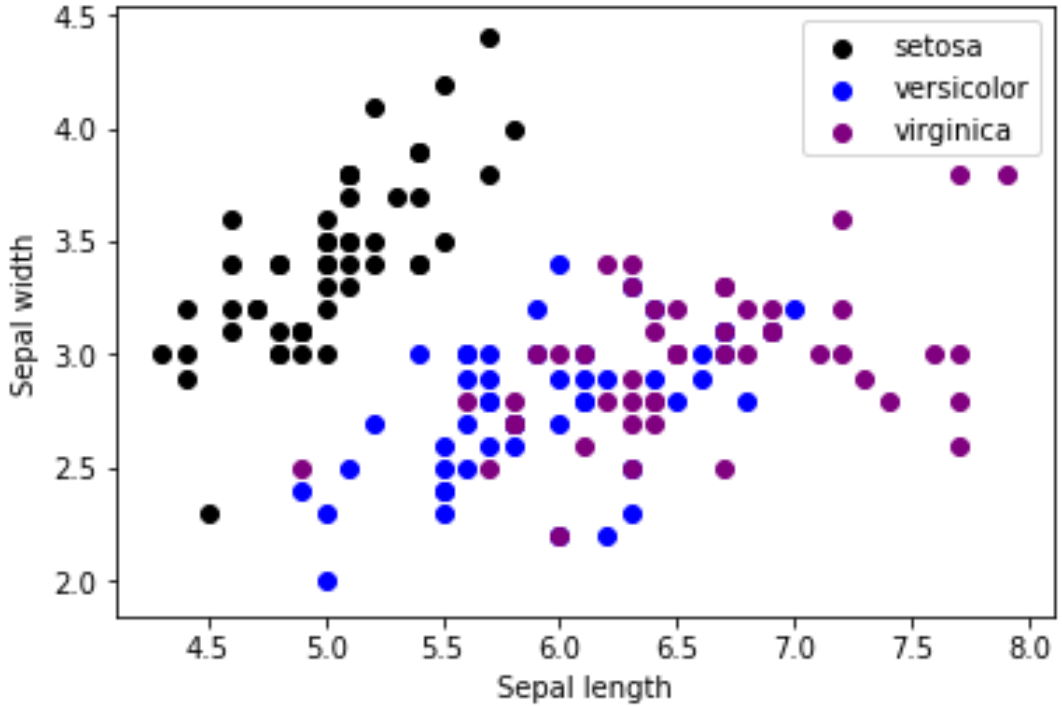
  Setosa, Versicolor and Verginica.

- It has four variables:
  - Sepal length and width
  - Petal length and width
- Which variables can I use to plot the data in two dimensional space?
- Let's try using the two features:

  Sepal length VS. Sepal width



Plotting the data points using Sepal Length vs Sepal Width

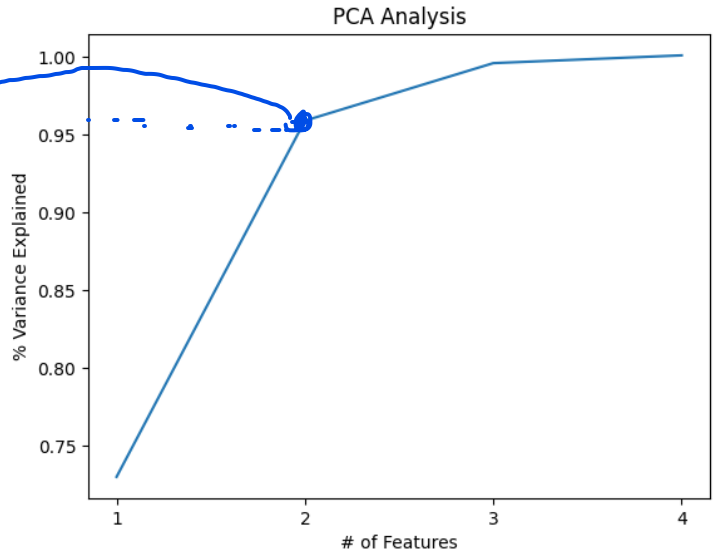


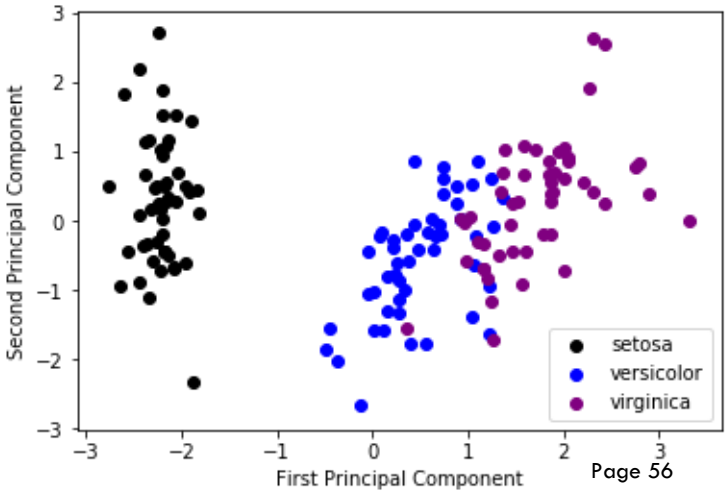
PCA on IRIS Dataset

- Let's now choose the best variables using PCA and then plot the data
- The eigenvalues are:

[0.728 0.230 0.037 0.005]

- The first two PCs represent 95.8% of the variance of the data
- Which means we can reduce the data into two dimensional spaces by eliminating PC3 and PC4





Review

W8 review: Clustering and Dimensionality Reduction

Objective

Learn techniques for unsupervised learning, with tools in Python.

Lecture

- Clustering algorithms
- Evaluating clustering
- Choosing k
- Principal Component Analysis

Readings

- Intro to Data Mining, Ch. 7 https://www-users.cse.umn.edu/~kumar001/dmbook/ch7_clustering.pdf
- Data Science from Scratch, Ch. 20

Exercises

- sklearn: clustering and PCA