Unsupervised Learning: Clustering

Some material adapted from slides by Andrew Moore, CMU. See http://www.autonlab.org/tutorials/ for a repository of Data Mining tutorials

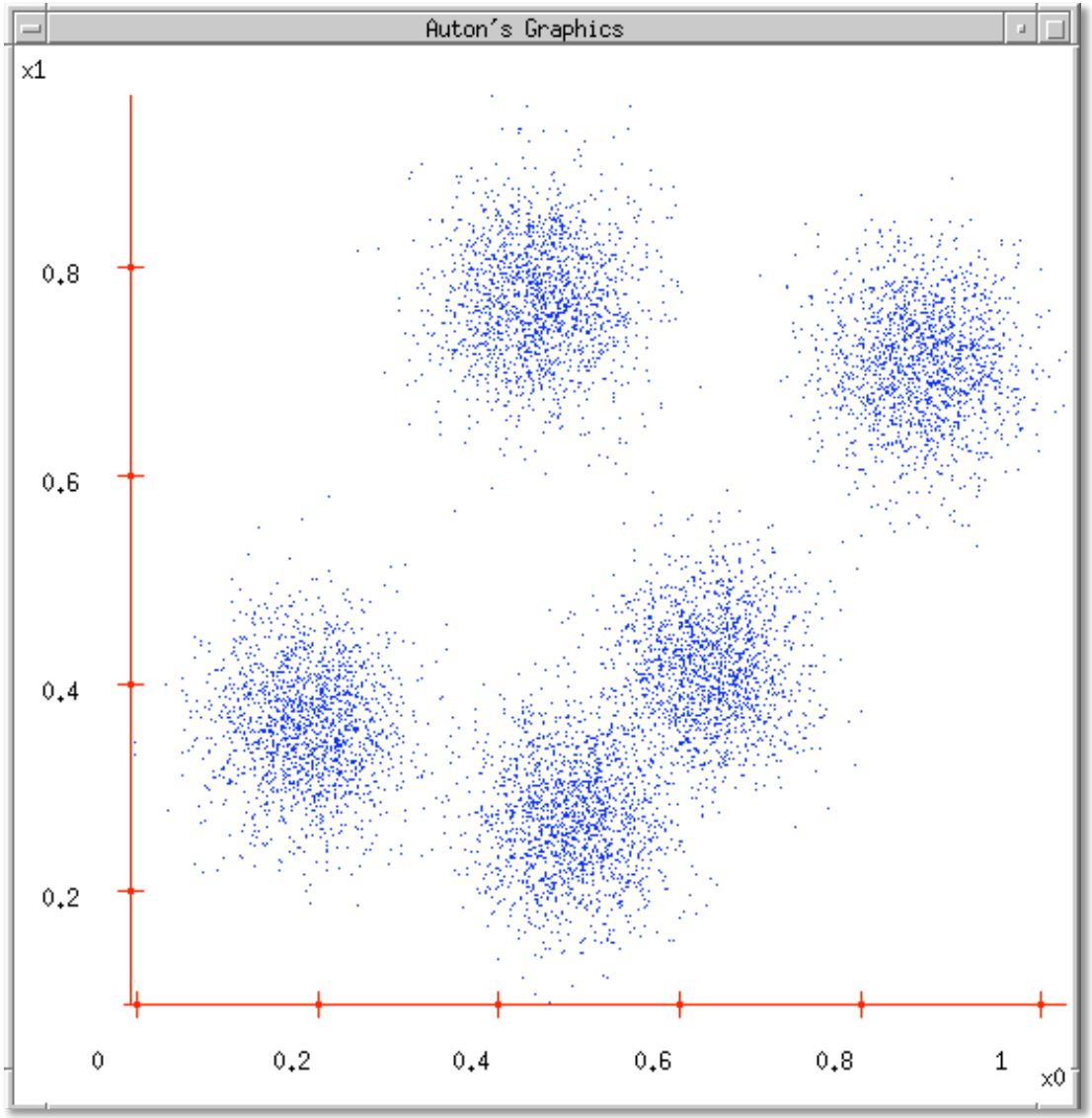
Unsupervised Learning

- Supervised learning used labeled data pairs (x, y) to learn a function f : X→Y.
- But, what if we don't have labels?
- No labels = **unsupervised learning**
- Only some points are labeled = **semi-supervised learning**
  - Getting labels may be expensive, so we only get a few
- **Clustering** is the unsupervised grouping of data points. It can be used for **knowledge discovery**

Clustering algorithms

- There are many clustering algorithms
- Clustering is typically done using a distance measure defined between instances
- The distance is defined in the instance feature space
- Agglomerative approach works bottom up:
  - Treat each instance as a cluster
  - Merge the two closest clusters
  - Repeat until the stop condition is met
- Top-down approach starts a cluster with all instances
  - Find a cluster to split into two or more smaller clusters
  - Repeat until stop condition met

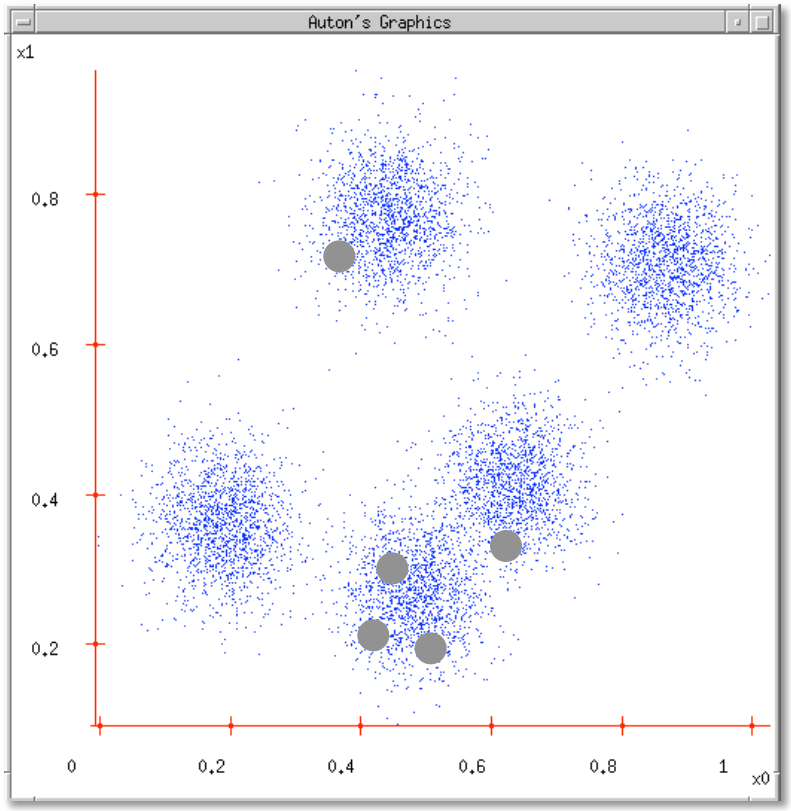
Clustering Data



K-Means Clustering

K-Means (k , data)

- Randomly choose k cluster center locations (centroids)
- Loop until convergence
  - Assign each point to the cluster of the closest centroid
  - Re-estimate the cluster centroids based on the data assigned to each
- Convergence: no point is assigned to a different cluster



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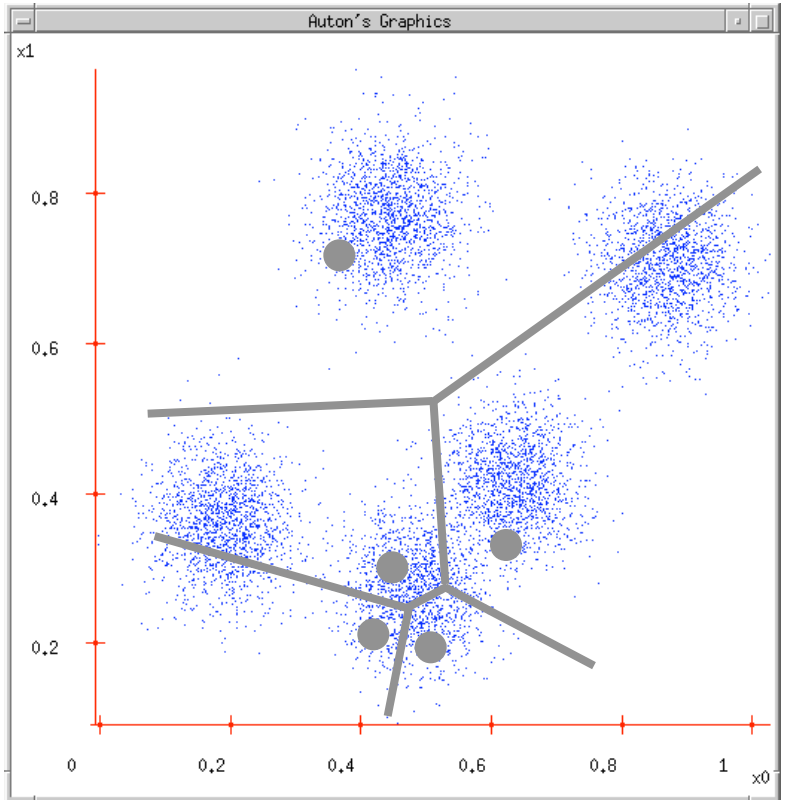

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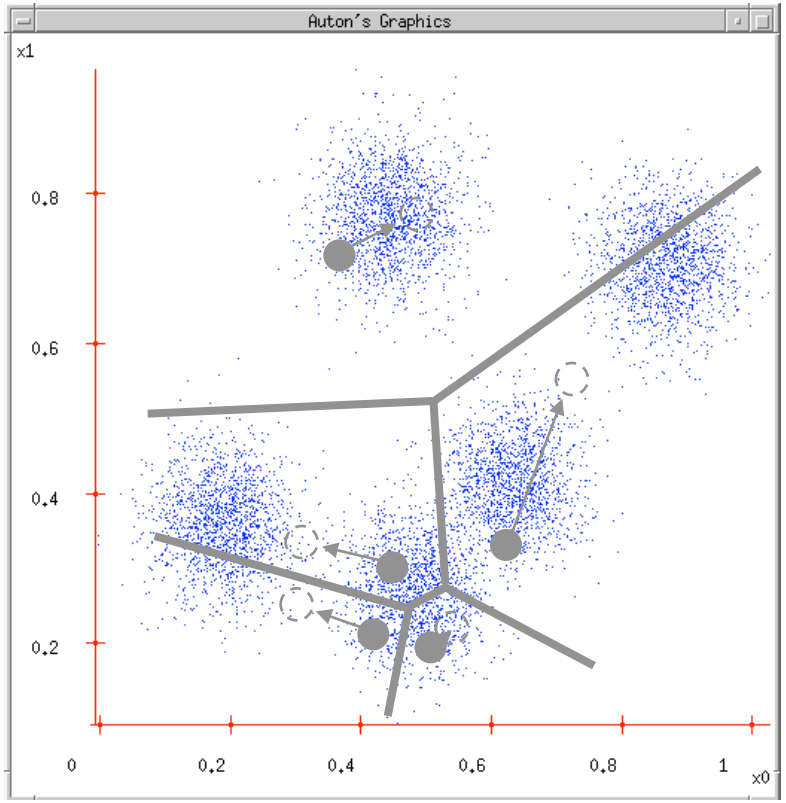

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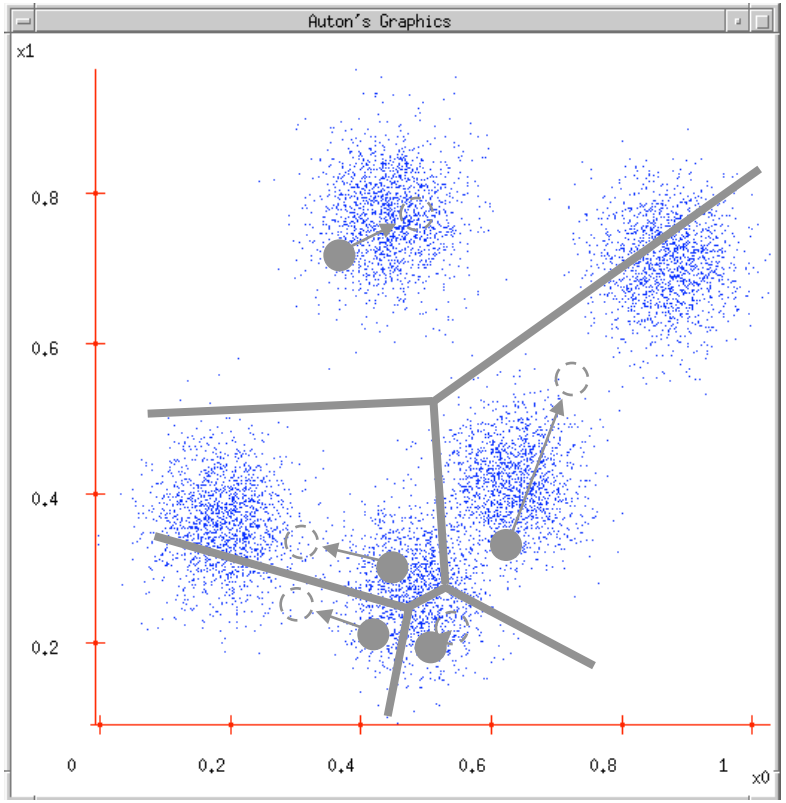
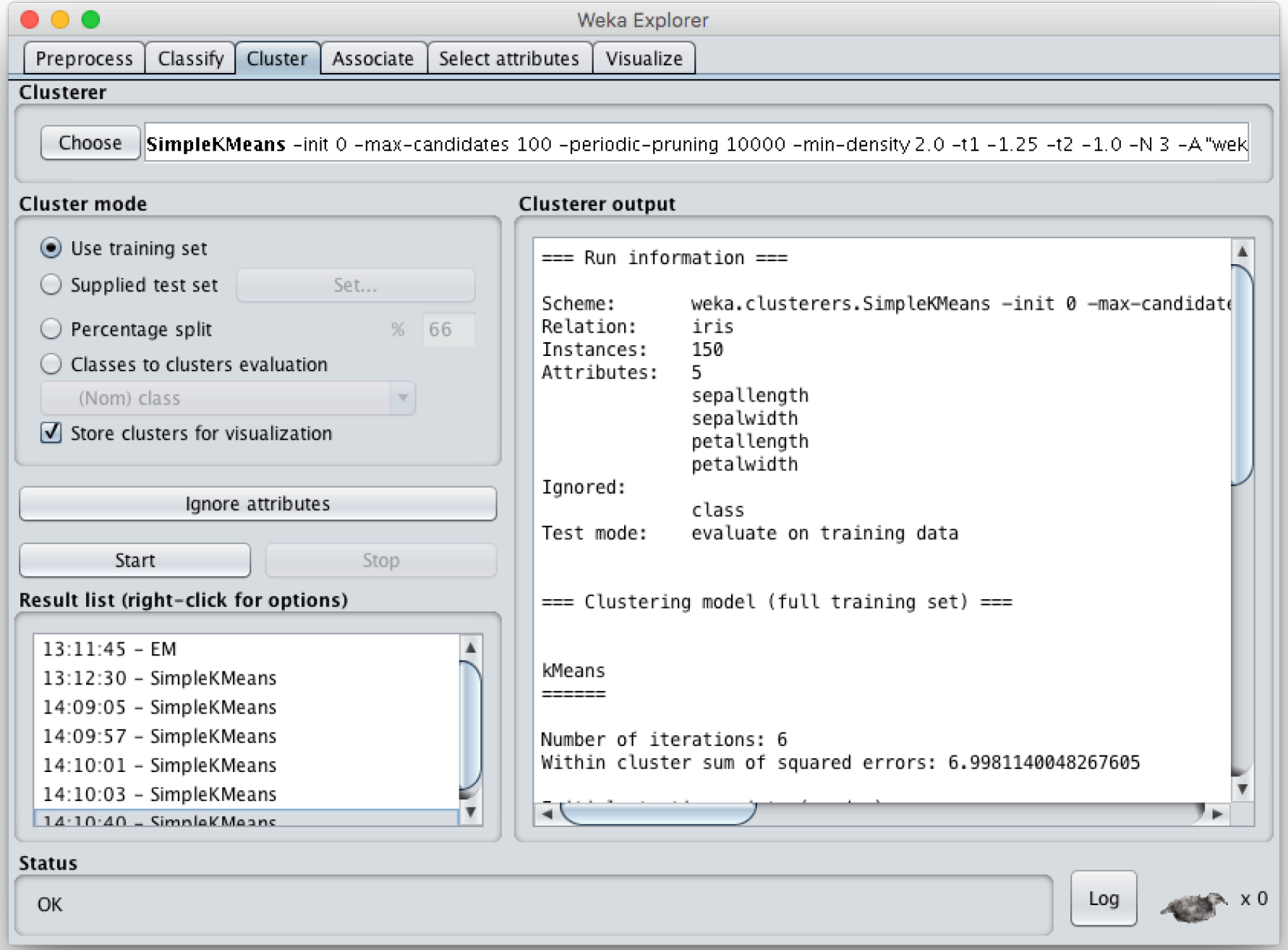



Weka Explorer
Preprocess
Classify
Cluster
Associate
Select attributes
Visualize
Clusterer
Choose
SimpleKMeans -init 0 -max-candidates 100 -periodic-pruning 10000 -min-density 2.0 -t1 -1.25 -t2 -1.0 -N 3 -A "wek
Cluster mode
Use training set
Supplied test set
Set...
Percentage split
% 66
Classes to clusters evaluation
(Nom) class
Store clusters for visualization
Ignore attributes
Start
Stop
Result list (right-click for options)
13:11:45 - EM
13:12:30 - SimpleKMeans
14:09:05 - SimpleKMeans
14:09:57 - SimpleKMeans
14:10:01 - SimpleKMeans
14:10:03 - SimpleKMeans
Clusterer output
=== Run information ===
Scheme: weka.clusterers.SimpleKMeans -init 0 -max-candidate
Relation: iris
Instances: 150
Attributes: 5
sepallength
sepalwidth
petallength
petalwidth
Ignored:
class
Test mode: evaluate on training data
=== Clustering model (full training set) ===
kMeans
======
Number of iterations: 6
Within cluster sum of squared errors: 6.9981140048267605
Status
OK
Log
x 0

Using scikit-learn for K-means clustering on Fisher's Iris dataset with a 3D graph

In [38]:
```
%matplotlib inline

from sklearn import datasets, cluster
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D

# Random seed chosen so cluster labeling corrsponds to the original y values
np.random.seed(2)
```

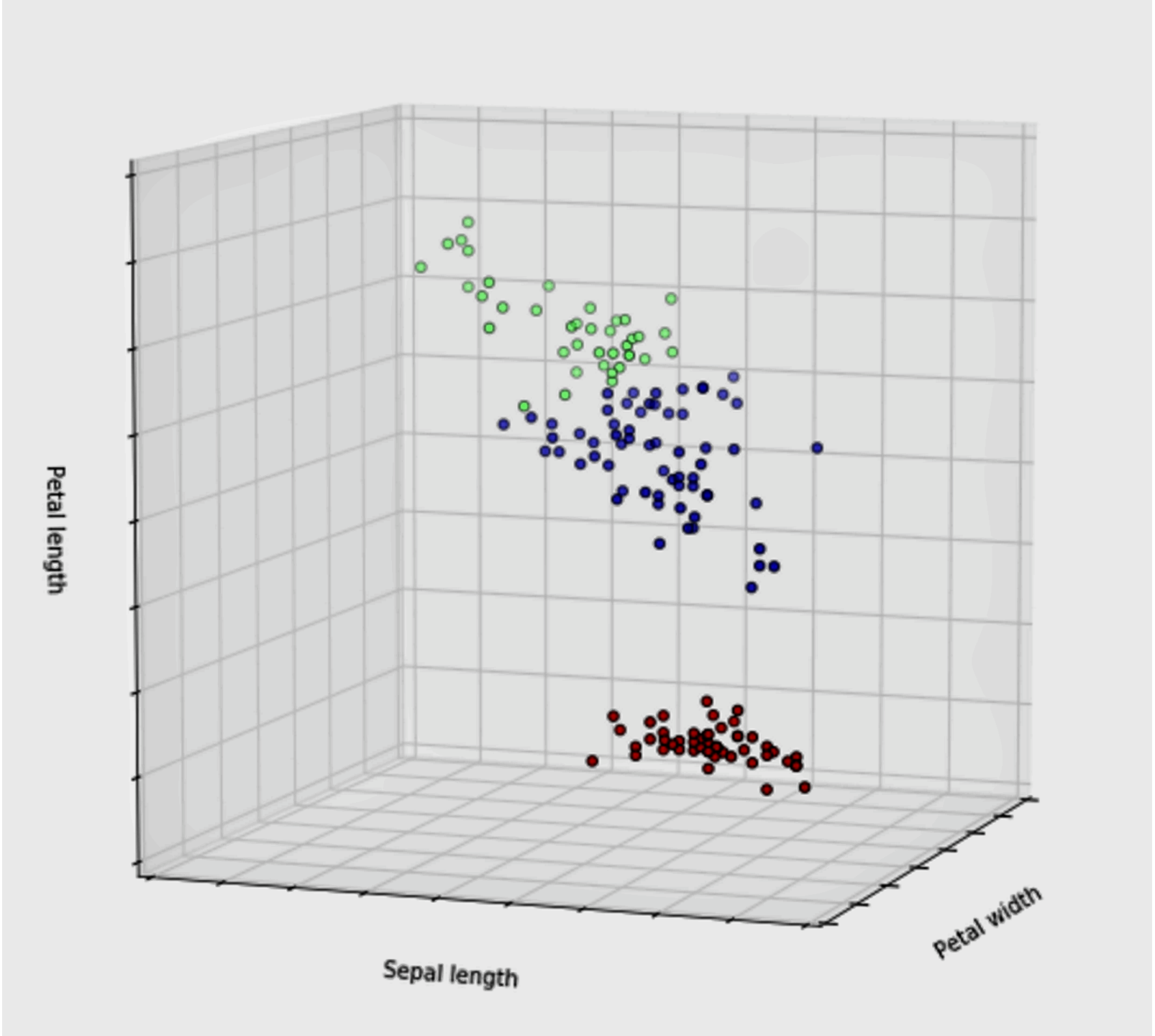
In [39]:
```
# load data
iris = datasets.load_iris()
X_iris = iris.data
y_iris = iris.target
```

In [40]:
```
# Form three clusters
k_means = cluster.KMeans(n_clusters=3)
k_means.fit(X_iris)
labels = k_means.labels_
```

In [41]:
```
# How many of the samples correctly labeled?
correct_labels = sum(y_iris == labels)

print("Result: %d of %d samples correctly labeled, inertia:%f." % (correct_labels, y
```

```
Result: 134 of 150 samples correctly labeled, inertia:78.940841.
```

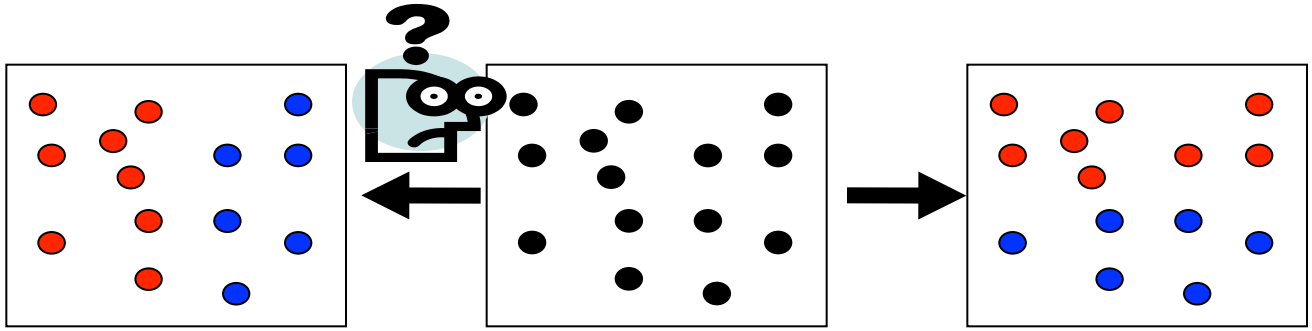

Petal length
Sepal length
Petal width

Problems with K-Means

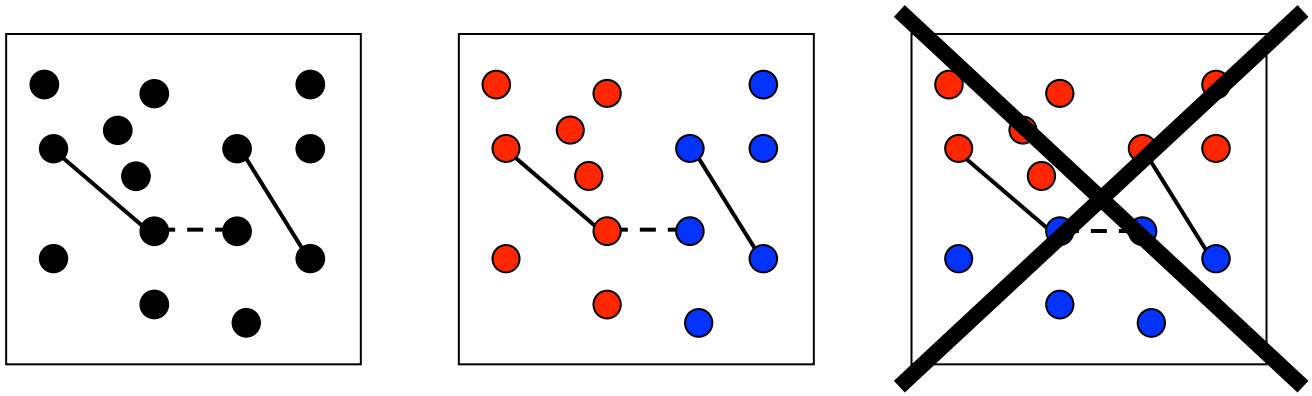
- Only works for numeric data (typical reals)
- ***Very*** sensitive to the initial points
  - Do many runs of k-Means, each with different initial centroids
  - Seed the centroids using a better method than random. (e.g., Farthest-first sampling)
- Must manually choose k
  - Learn the optimal k for the clustering. (Note that this requires a performance measure)

Problems with K-Means

- How do you tell it which clustering you want?

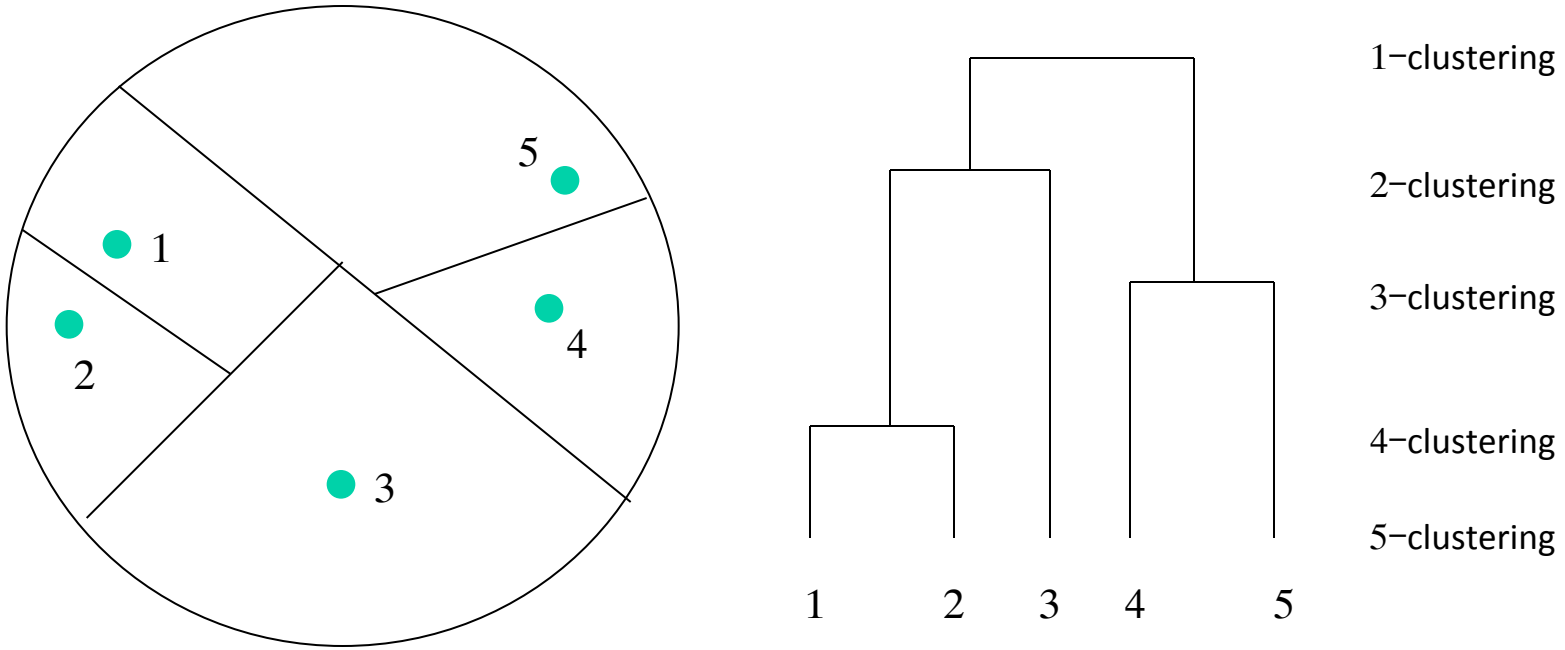


– Constrained clustering techniques



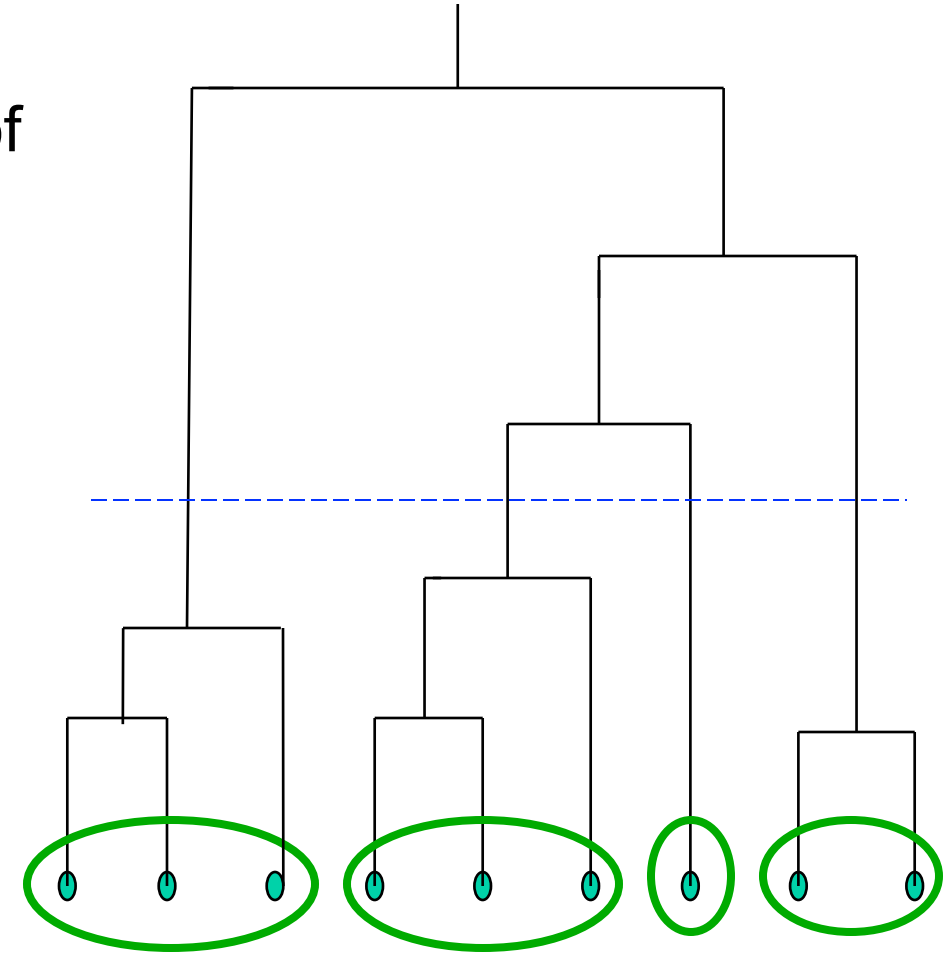
Hierarchical Clustering

Recursive partitioning/merging of a data set



Dendogram

- Represents all partitionings of the data
- We can get a K clustering by looking at the **connected** components at any given level
- Frequently binary dendograms, but n-ary dendograms are easy to obtain with minor changes to algorithms

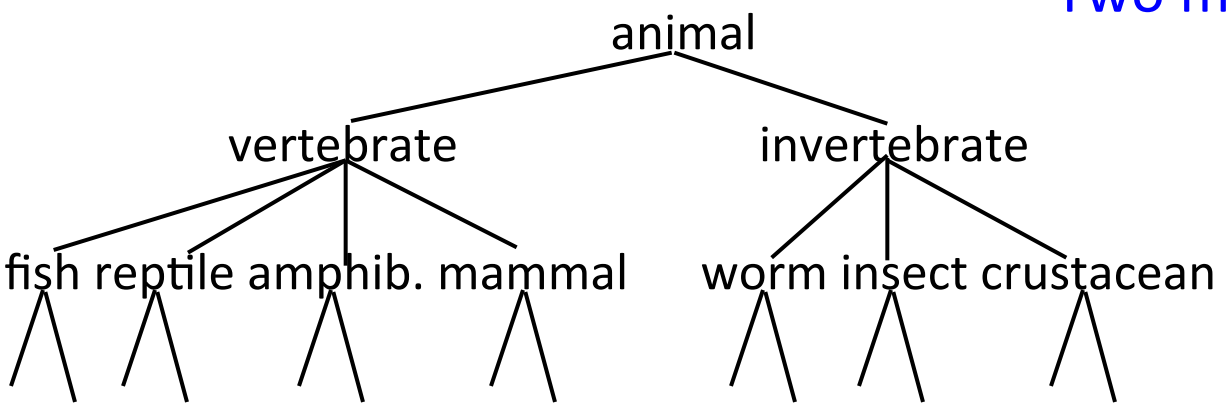


Advantages of hierarchical clustering

- Don't need to specify the number of clusters
- Good for data visualization
  - See how the data points interact at many levels
  - Can view the data at multiple levels of granularity
  - Understand how all points interact
- Specifies all of the K clusterings/partitions

Hierarchical Clustering

- Common in many domains
  - Biologists and social scientists
  - Gene expression data
  - Document/web page organization
    - DMOZ
    - Yahoo directories

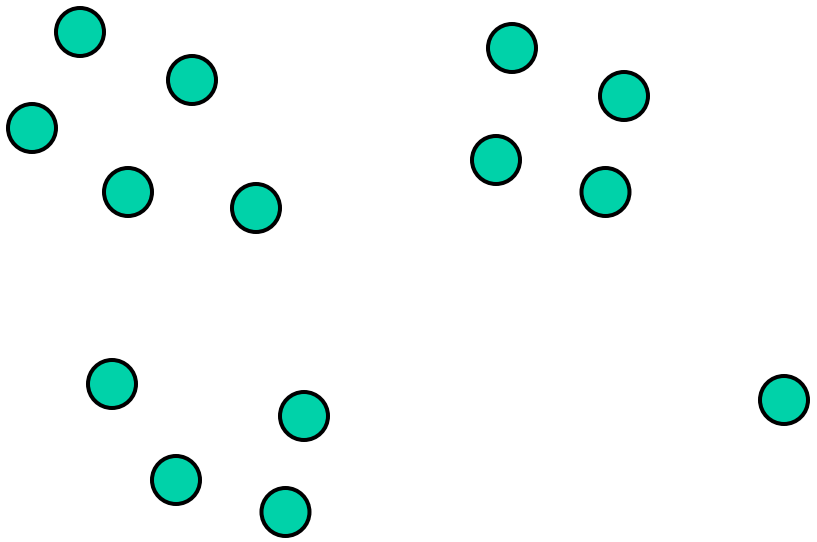


Two main approaches…

Divisive hierarchical clustering

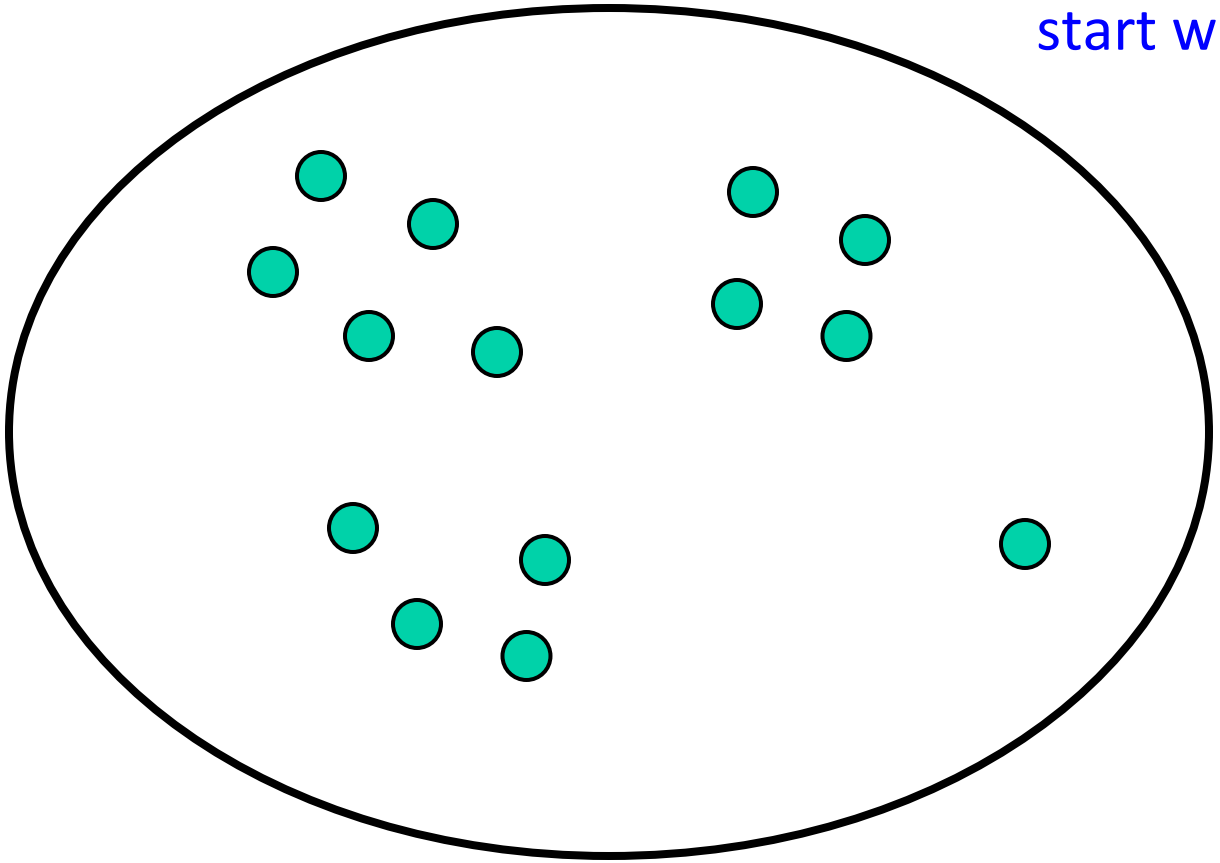
- Top-down
- Finding the best partitioning of the data is generally exponential in time
- Common approach:
  - Let **C** be a set of clusters
  - Initialize **C** to be the one-clustering of the data
  - While there exists a cluster *c* in **C**
    - remove *c* from **C**
    - partition *c* into 2 clusters using a flat clustering algorithm, c_1 and c_2
    - Add to c_1 and c_2 **C**
- Bisecting k-means

Divisive clustering



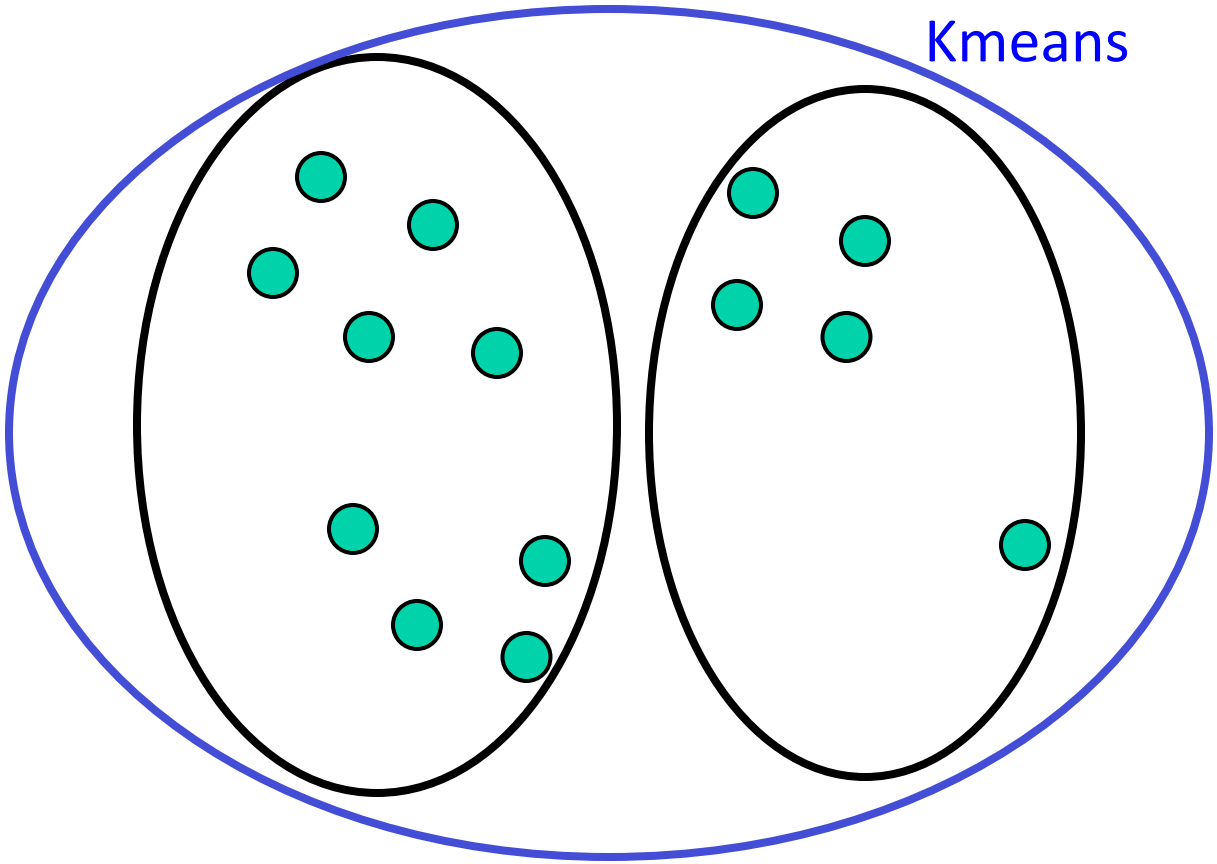
Divisive clustering

start with one cluster

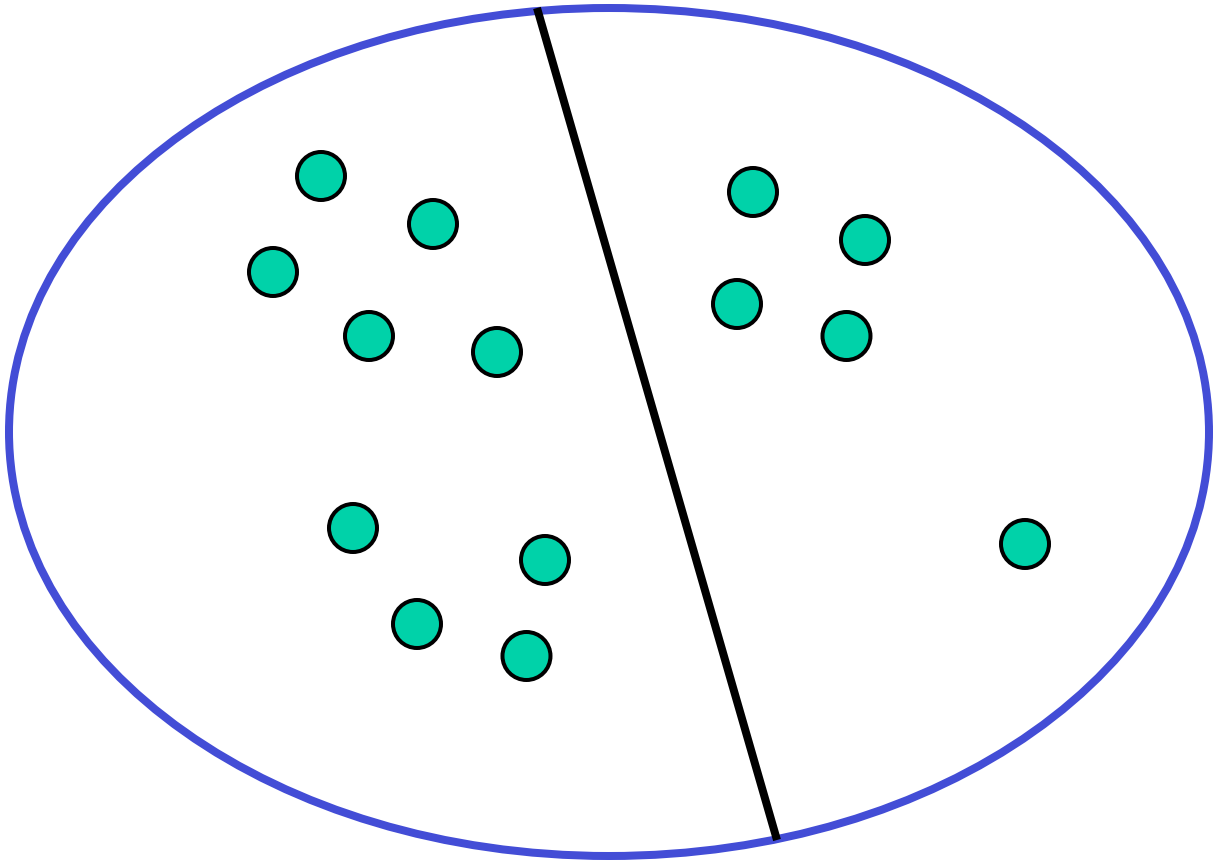


Divisive clustering

split using flat clustering, e.g. Kmeans

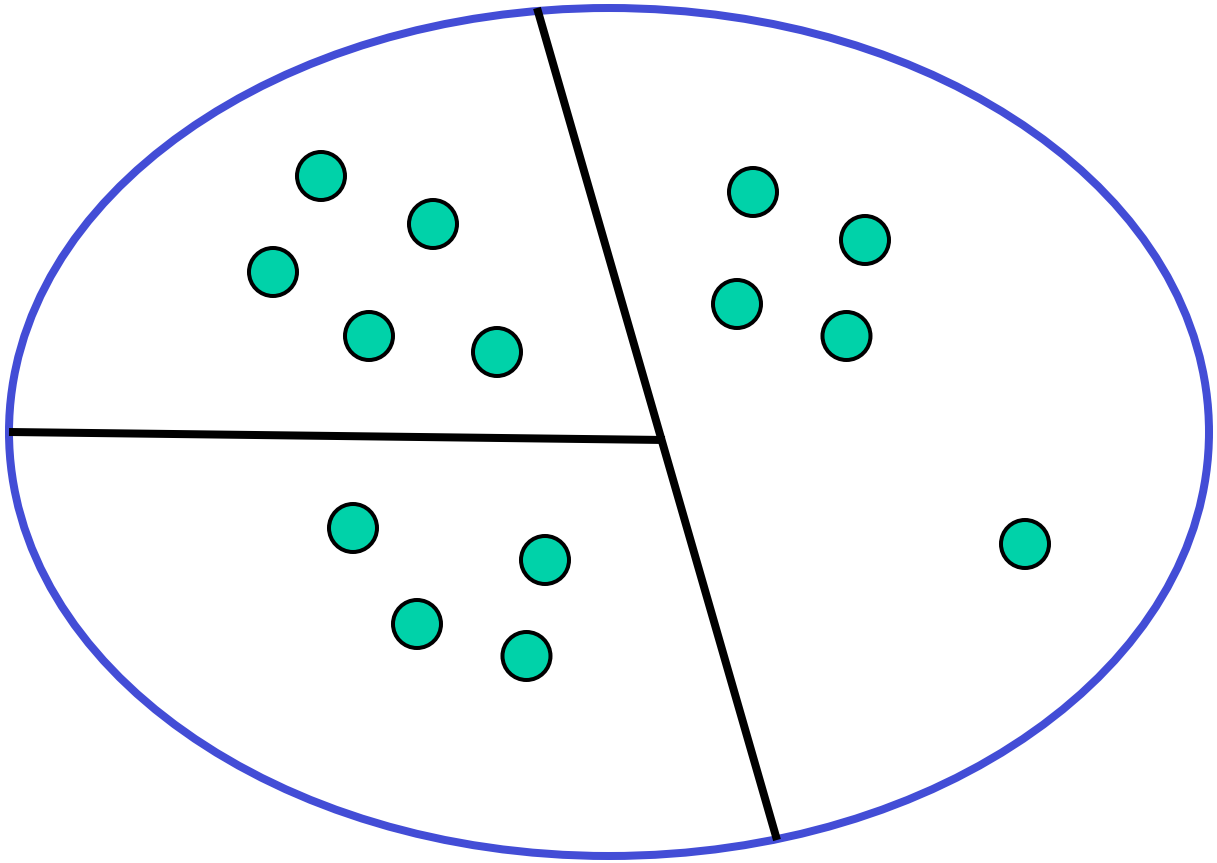


Divisive clustering



Divisive clustering

split using flat clustering



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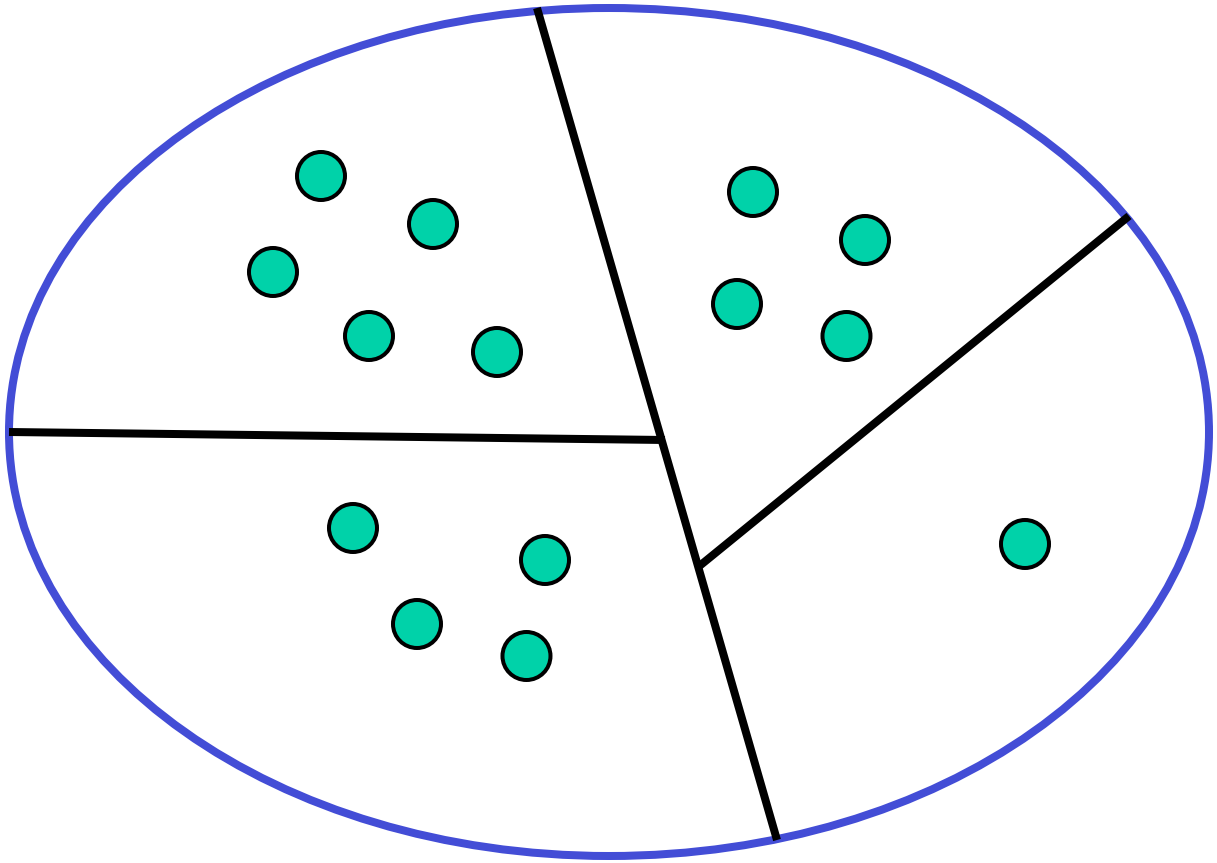

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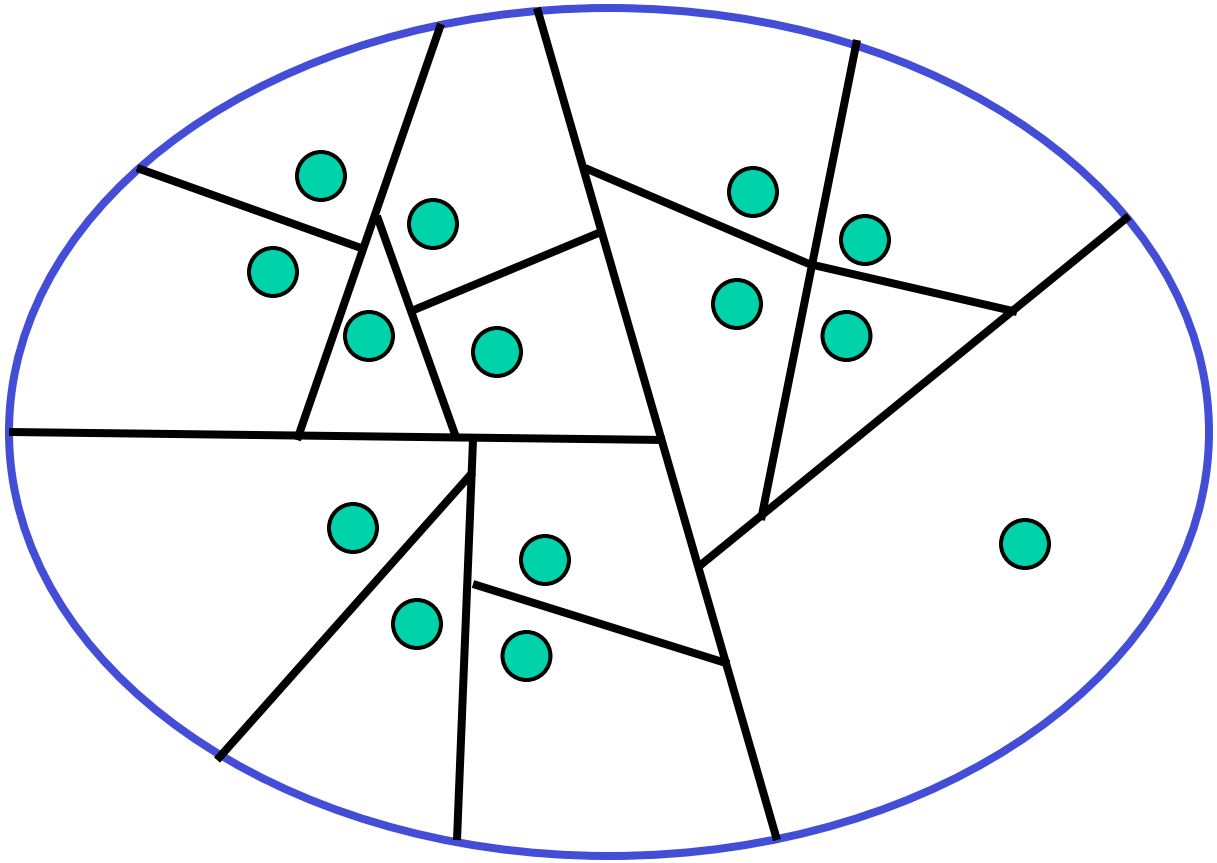


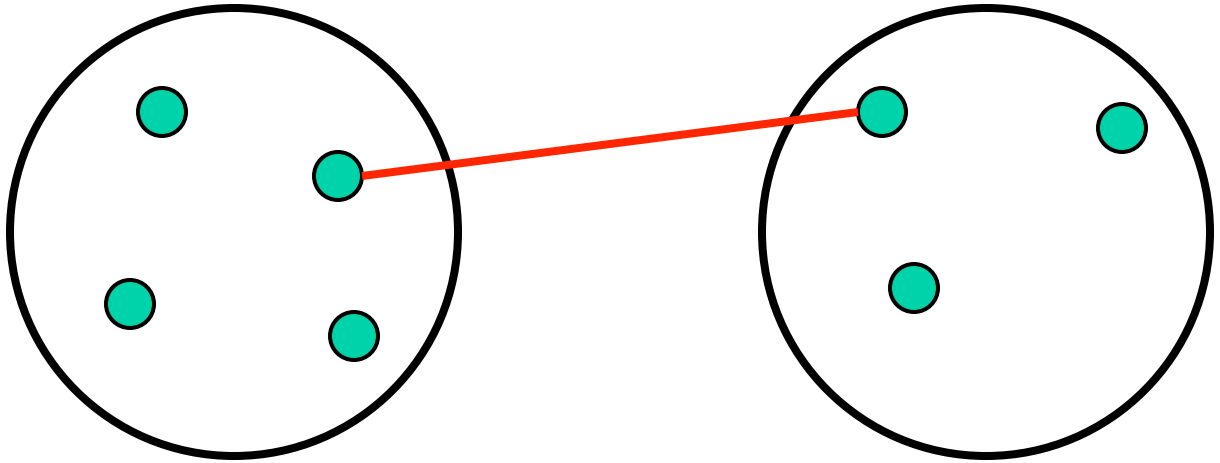
Hierarchical Agglomerative Clustering

- Let **C** be a set of clusters
- Initialize **C** to all points/docs as separate clusters
- While **C** contains more than one cluster
  - find c_1 and c_2 in **C** that are closest together
  - remove c_1 and c_2 from **C**
  - merge c_1 and c_2 and add resulting cluster to **C**
- History of merging forms a binary tree or hierarchy
- Q: How to measure distance between clusters?

Distance between clusters

Single-link

- Similarity of the *most* similar (single-link)



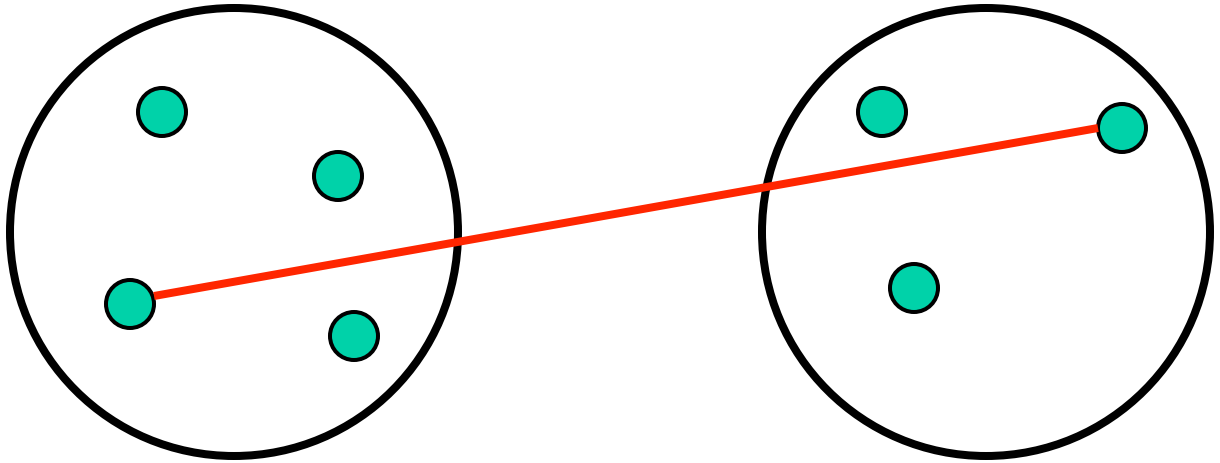
$$\max_{l \in L, r \in R} sim(l,r)$$

Distance between clusters

Complete-link

- Similarity of the "furthest" points, the *least* similar

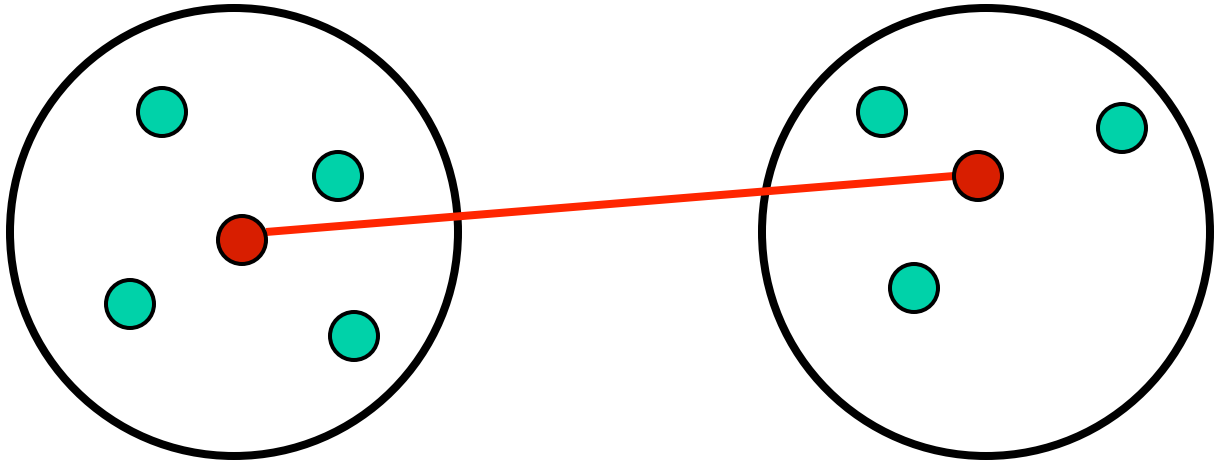
$$\min_{l \in L, r \in R} sim(l, r)$$



Why are these "local" methods used? efficiency

Distance between clusters

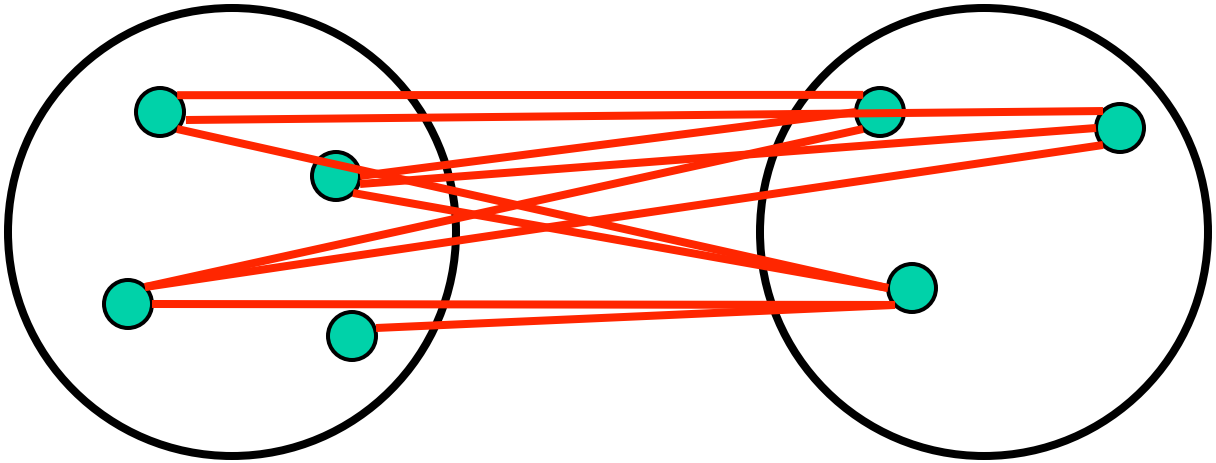
- **Centroid**
  - Clusters whose centroids (centers of gravity) are the most similar



$$\left\|\mu(L) - \mu(R)\right\|^2$$

Distance between clusters

- **Average-link**
  - Average similarity between all pairs of elements



$$\frac{1}{|L| \cdot |R|} \sum_{x \in L, y \in R} \|x - y\|^2$$