CS 4602

Introduction to Machine Learning

Clustering

Instructor: Po-Chih Kuo

Roadmap

- Introduction and Basic Concepts
- Regression
- Bayesian Classifiers
- Decision Trees
- Linear Classifier
- Neural Networks
- Deep learning
- Convolutional Neural Networks
- The others
- KNN
- Clustering
- Data Exploration & Dimensionality reduction
- Model Selection and Evaluation

Outline

- Why clustering?
- Choosing (dis)similarity measures
- Clustering algorithms

Ref: Slides from Georg Gerber

What is clustering?

- A way of grouping together data samples that are ***similar*** according to some criteria
- A form of ***unsupervised learning***
  - Don’t need testing data demonstrating how the data should be grouped together
- It’s a method of ***exploratory data analysis (EDA)***
  - looking for patterns or structures in the data that are of interest
  - no explicit labels; the clusters may need further interpretation.

Applications

- Streaming Services
    - To identify viewers who have similar behavior.

Minutes watched per day

Total viewing sessions per week

Number of unique shows viewed per month

More Applications

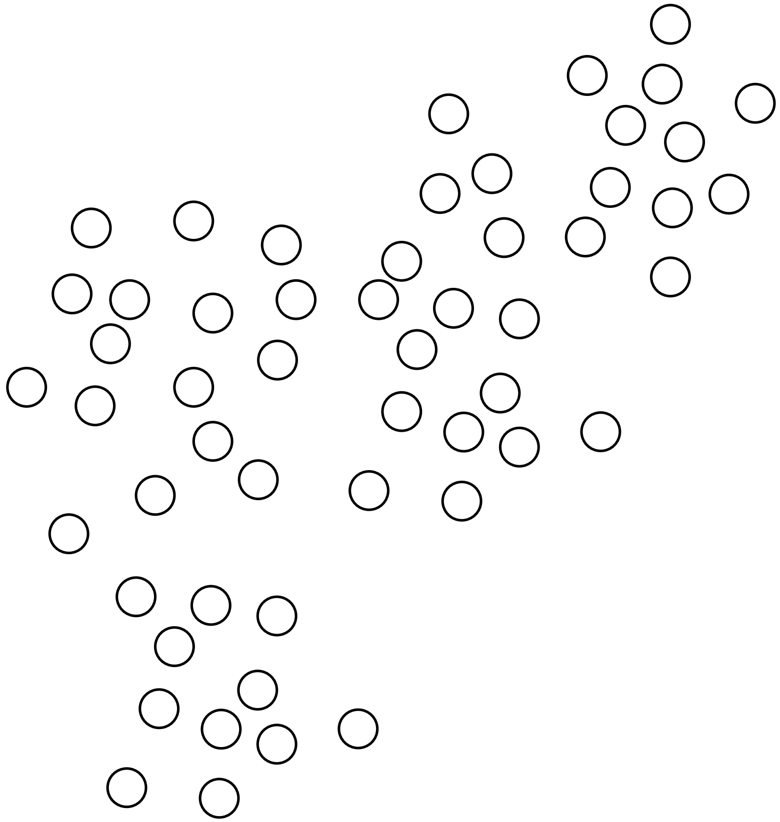
Marketing & Retail	Customer Segmentation	Group customers based on behavior, demographics, or preferences for targeted marketing.
Computer Vision	Image Segmentation	Segment images into objects or regions (e.g., tumor detection in medical imaging).
NLP	Document Clustering	Group similar documents or articles for topic modeling or news categorization.
Cybersecurity	Anomaly Detection	Detect unusual patterns such as fraud or network intrusions.
Social Media	Social Network Analysis	Identify communities or influencer groups within networks.
Bioinformatics	Gene Expression Analysis	Cluster genes with similar expression patterns for disease understanding.
Entertainment	Recommender Systems	Suggest movies, music, or products based on user behavior.
Healthcare	Patient Segmentation	Group patients by medical history or symptoms for personalized treatment.
Psychology	Behavioral Analysis	Cluster individuals based on behavioral data to understand user preferences.
Education	Student Clustering	Group students by learning styles or performance for personalized education.

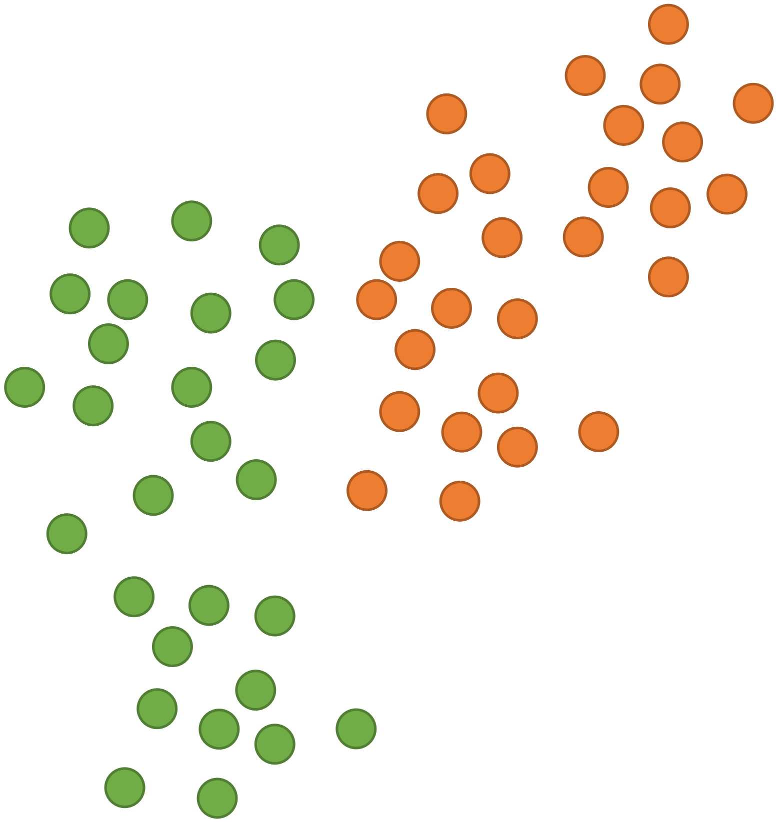
Group by features (Column clustering)

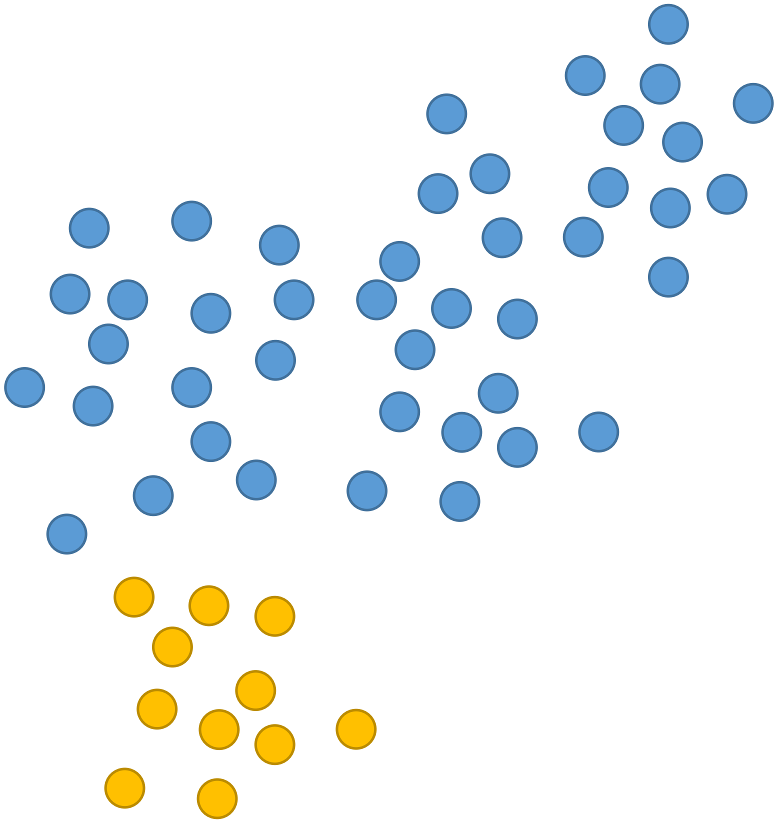
Example	Attributes										Target
	Alt.	Bar	Fri	Hun	Pat	Price	Rain	Res	Type	Est.	Wait
X_1	T	F	F	T	Some	$$$	F	T	French	0-10	[redacted]
X_2	T	F	F	T	Full	$	F	F	Thai	30-60	[redacted]
X_3	F	T	F	F	Some	$	F	F	Burger	0-10	[redacted]
X_4	T	F	T	T	Full	$	F	F	Thai	10-30	[redacted]
X_5	T	F	T	F	Full	$$$	F	T	French	>60	[redacted]
X_6	F	T	F	T	Some	$$	T	T	Italian	0-10	[redacted]
X_7	F	T	F	F	None	$	T	F	Burger	0-10	[redacted]
X_8	F	F	F	T	Some	$$	T	T	Thai	0-10	[redacted]
X_9	F	T	T	F	Full	$	T	F	Burger	>60	[redacted]
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10-30	[redacted]
X_{11}	F	F	F	F	None	$	F	F	Thai	0-10	[redacted]
X_{12}	T	T	T	T	Full	$	F	F	Burger	30-60	[redacted]

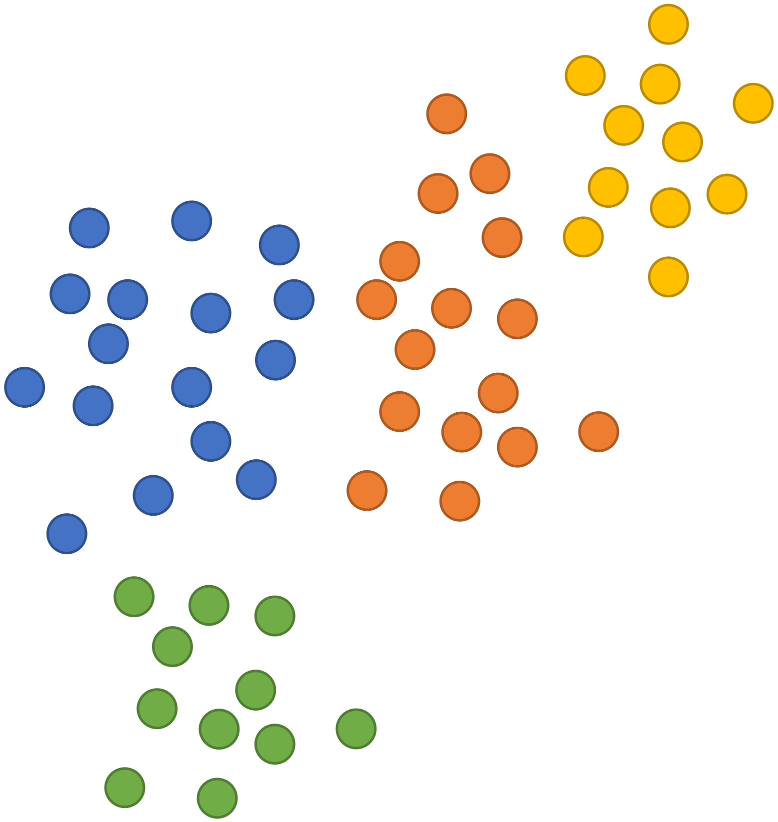
Group by instances (Row clustering)

How to cluster the data?









There is no single correct answer!

What similarity is required for items to be placed in the same cluster?

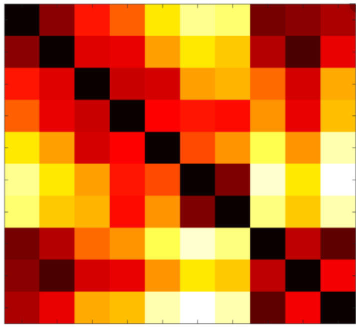
Outline

- Motivation
- Choosing (dis)similarity measures
  - **a critical step in clustering**
- Clustering algorithms

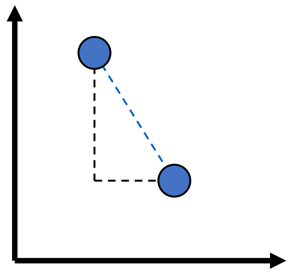
Ref: Slides from Georg Gerber

How do we define **(dis)similarity**?

- The goal is to group together "**similar**" data
- It depends on what we want to find or emphasize in the data;
- The similarity measure is often more important than the clustering algorithm used
- This is usually a ***pair-wise*** measure



Euclidean distance



$$d_{euc}(\mathbf{x},\mathbf{y}) = \sqrt{\sum_{i=1}^{n}(x_i - y_i)^2}$$

- Here *n* is the number of dimensions in the data vector. For instance:
  - Number of features (when clustering instances)
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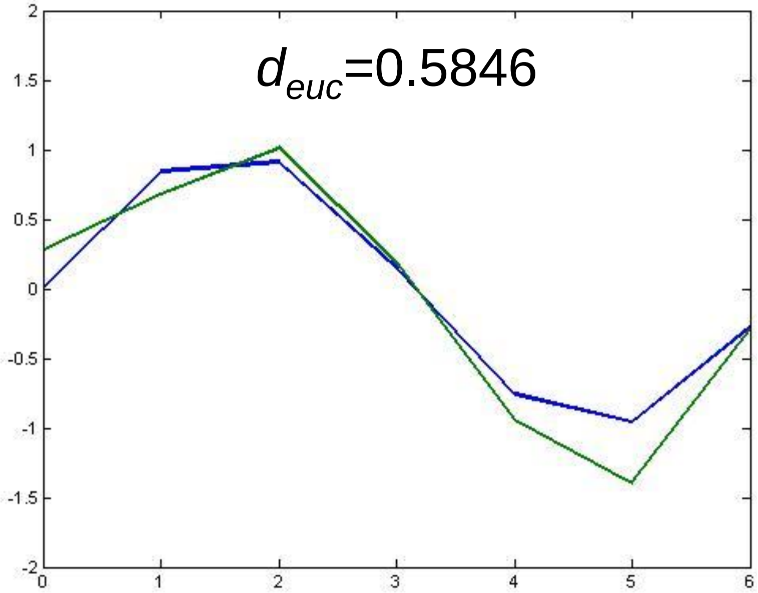
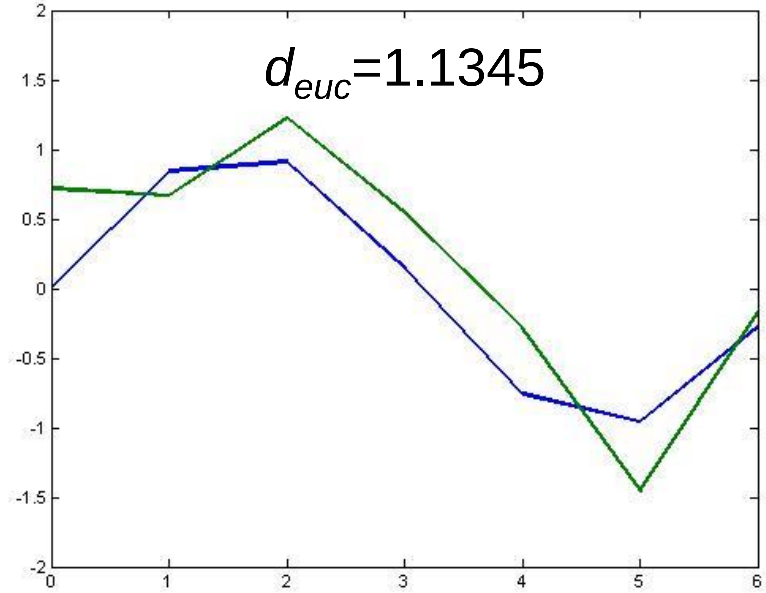
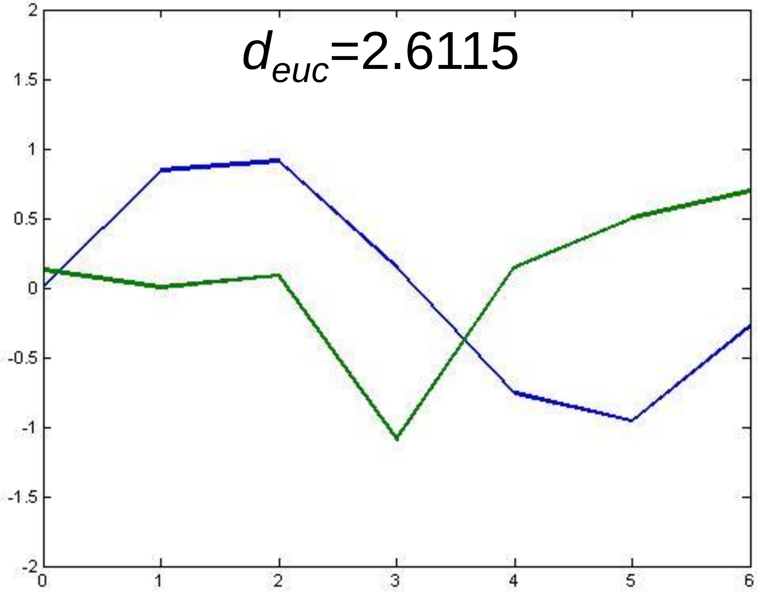
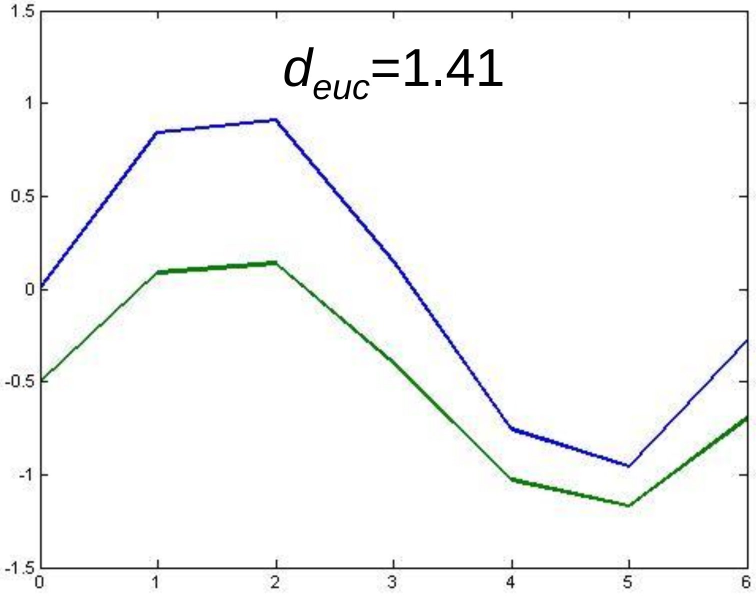


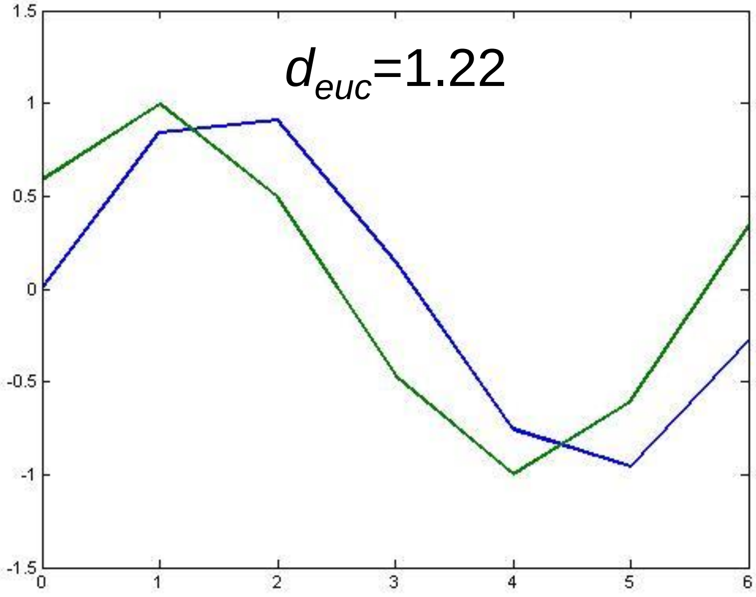




These examples of Euclidean distance match our intuition of dissimilarity well…

But what about these?

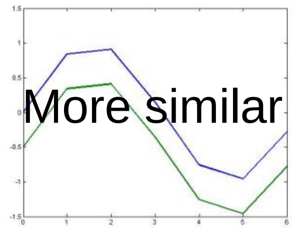


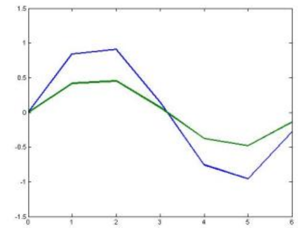


What might be going on with the data profiles on the left? On the right?

Pearson Correlation

- We might care more about the shape of data profiles rather than the magnitudes





- We can make the data have mean = 0 and std = 1

$$\rho(\mathbf{x},\mathbf{y}) = \frac{\sum_{i=1}^{n}(x_i-\bar{x})(y_i-\bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i-\bar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i-\bar{y})^2}}$$

$$\bar{x} = \frac{1}{n}\sum_{i}^{n} x_i$$

$$\bar{y} = \frac{1}{n}\sum_{i}^{n} y_i$$

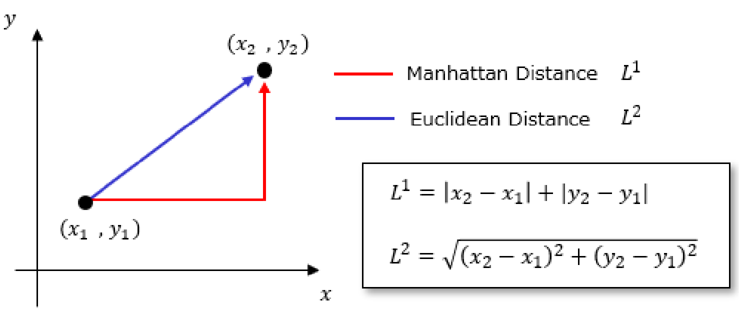
Pearson Correlation

- Pearson correlation is a measure that is invariant to scaling and shifting of the data values
- Always between –1 and +1
- We can easily make it into a dissimilarity measure:

$$d_p = \frac{1 - \rho(\mathbf{x}, \mathbf{y})}{2}$$

Other measures

- Manhattan distance (or Cityblock, or L1), cosine distance



Manhattan is preferred over Euclidean distance:

1. High dimensional data.
2. Data points are not evenly distributed across all dimensions.

Outline

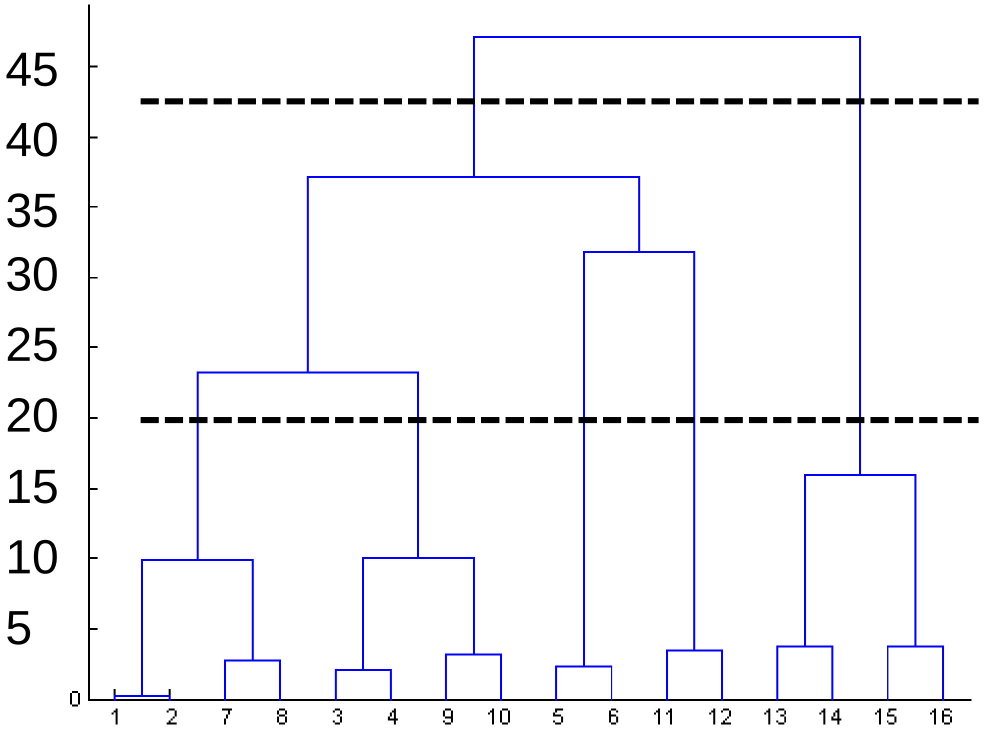
- Motivation
- Choosing (dis)similarity measures – **a critical step in clustering**
- Clustering algorithms
  - Hierarchical clustering
  - K-means

Ref: Slides from Georg Gerber

Hierarchical Clustering

- Start with every data point in a separate cluster
- Keep merging the most similar pairs of data points/clusters until we have one big cluster left
- A bottom-up method

Hierarchical Clustering (cont.)



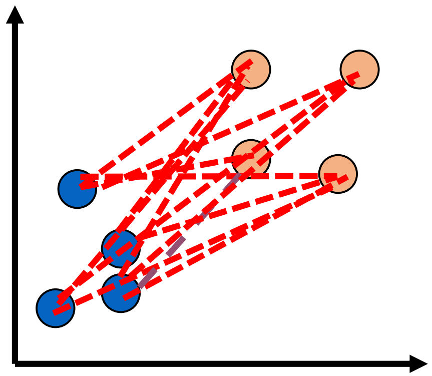
- This produces a binary tree or ***dendrogram***
- The final cluster is the root and each data item is a leaf
- The height of the bars indicate how close the items are

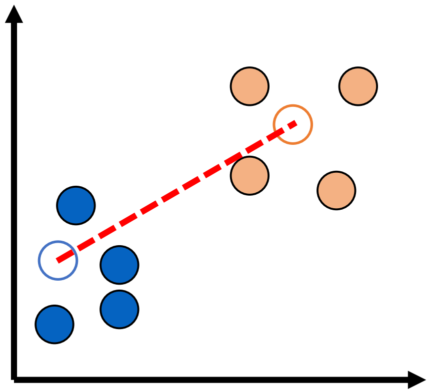
Linkage in Hierarchical Clustering

- We already know about distance measures between data items, but what about between a data item and a cluster or between two clusters?
- We just treat a data point as a cluster with a single item, so our only problem is to define a ***linkage*** method between clusters

Average Linkage

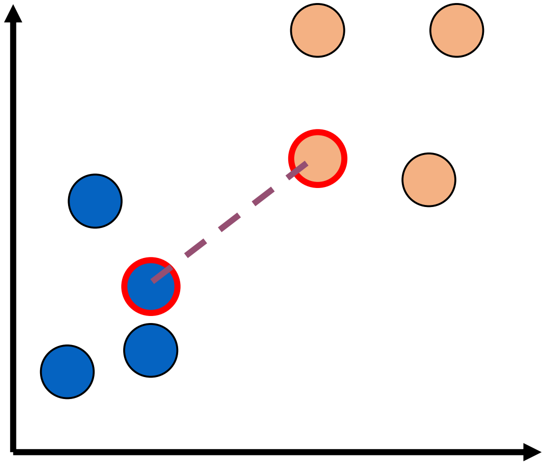
- Average linkage is defined as follows:
  - Each cluster c_i is associated with a mean vector μ_i which is the mean of all the data items in the cluster
  - The distance between two clusters c_i and c_j is then just $d(\mu_i, \mu_j)$





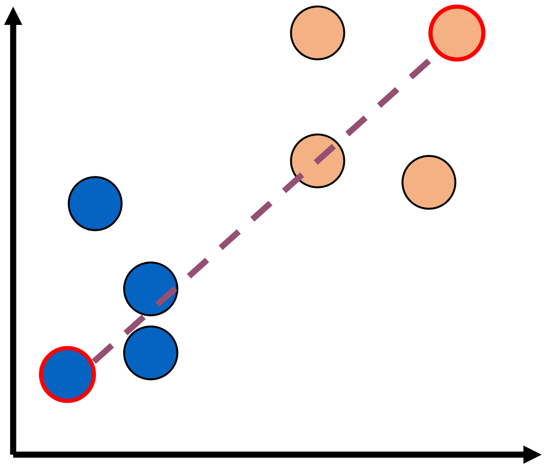
Single Linkage

- The **minimum** of all pairwise distances between points in the two clusters
- Tends to produce **loose** clusters



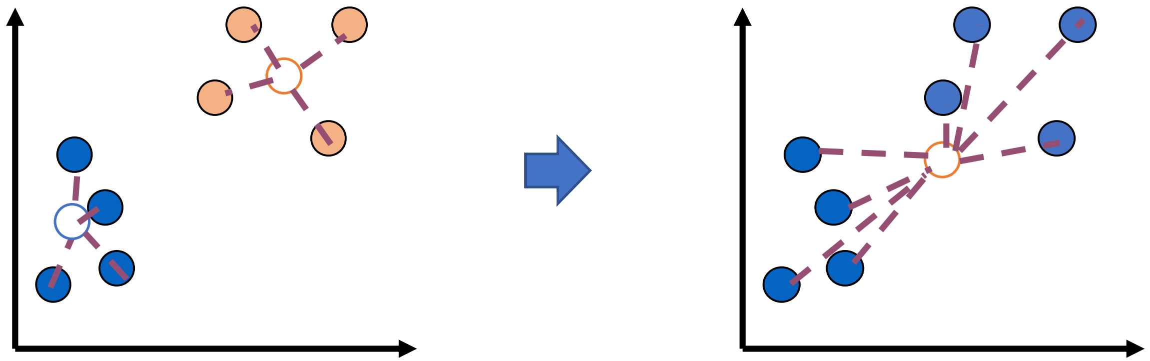
Complete Linkage

- The **maximum** of all pairwise distances between points in the two clusters
- Tends to produce **tight** clusters

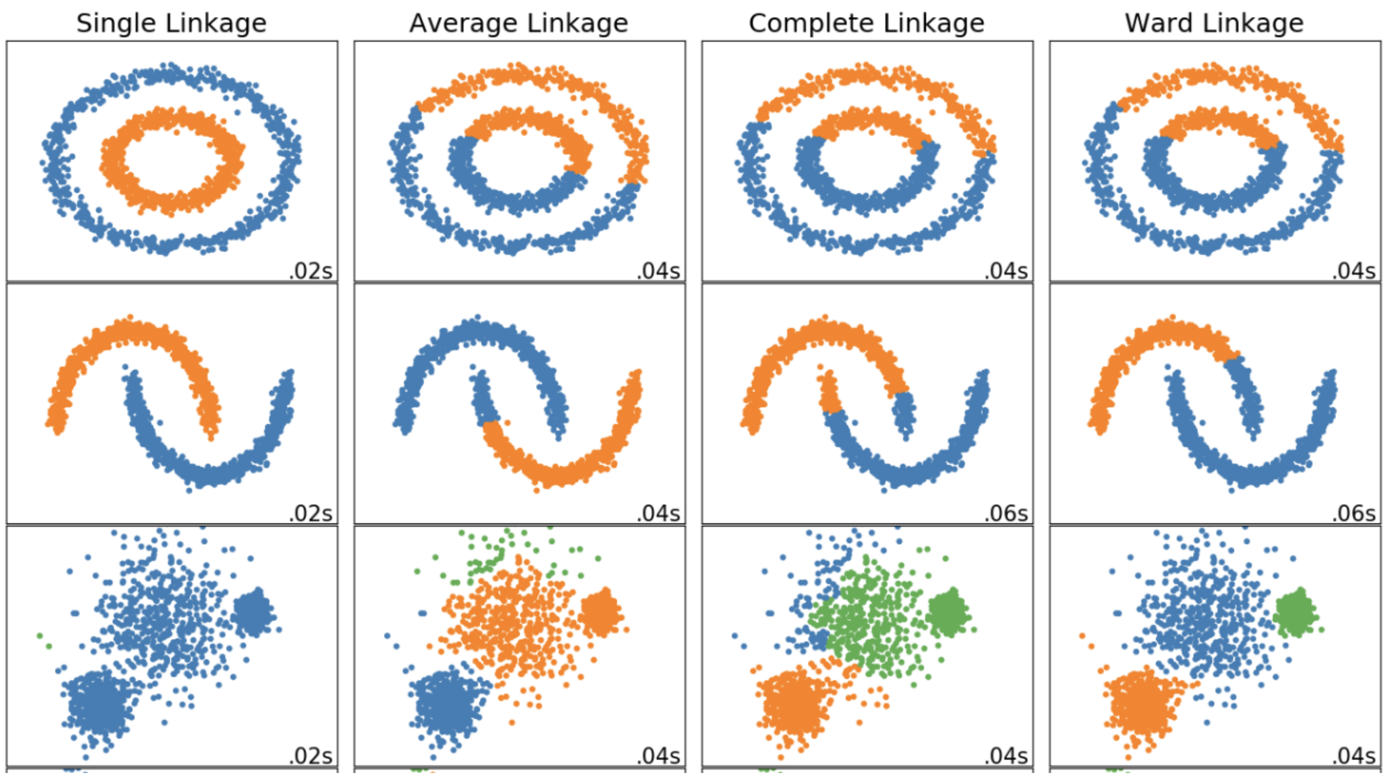


Ward’s Method

- Consider merging two clusters, how does it change the total distance from centroids?



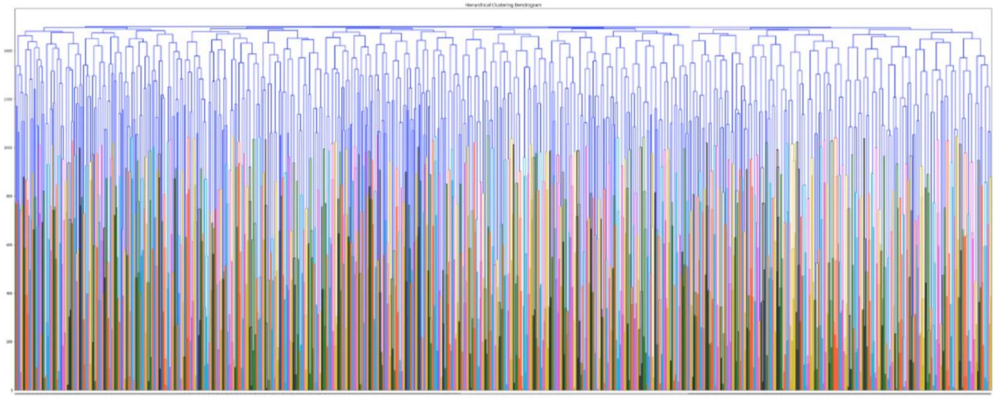
1. Find the centroid of each cluster.
2. Calculate the distance between each object and its cluster’s centroid.
3. Calculate the sum of squared differences from Step 2.
4. Add up all the sums from Step 3.



Single Linkage
Average Linkage
Complete Linkage
Ward Linkage
.02s
.04s
.04s
.04s
.02s
.04s
.06s
.06s
.02s
.04s
.04s
.04s

Hierarchical Clustering Issues

- Distinct clusters are not produced → No need to present the number of clusters
- There are methods for producing distinct clusters, but these usually involve specifying arbitrary **cutoff values**
- Heavy computation



Outline

- Motivation
- Choosing (dis)similarity measures – **a critical step in clustering**
- Clustering algorithms
  - Hierarchical clustering
  - K-means

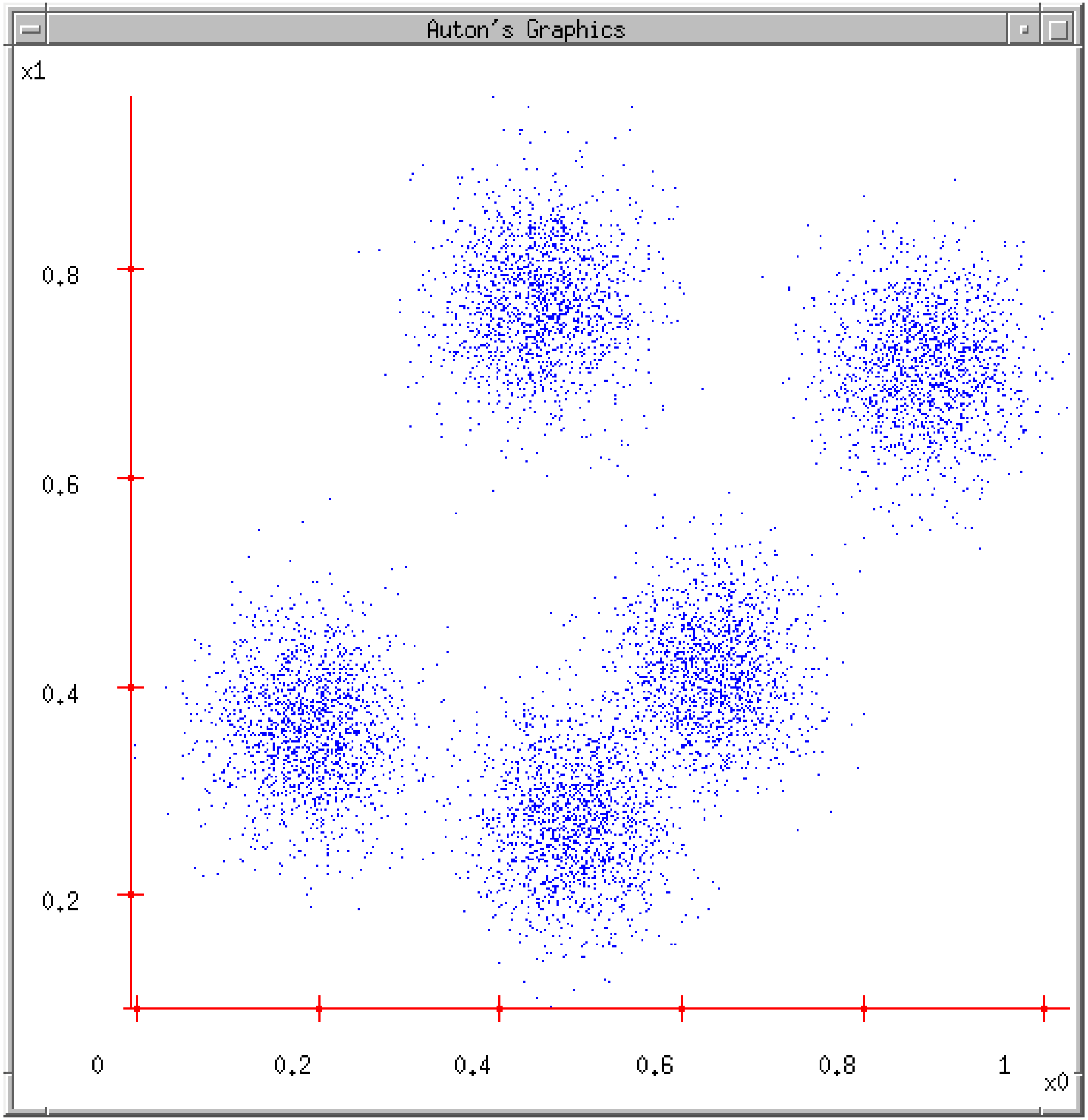
Ref: Slides from Georg Gerber

K-means Clustering

- Choose the number of clusters *k*
- Initialize cluster centers $\mu_1,\ldots \mu_k$
  - Randomly pick *k* data points and set cluster centers to these points
- For each data point, compute the cluster center it is closest to (using a distance measure) and assign the data point to this cluster
- Re-compute cluster centers (mean of data points in the cluster)
- **Stop when there are no new re-assignments**

K-means

1. Ask user how many clusters they'd like. *(e.g. k=5)*



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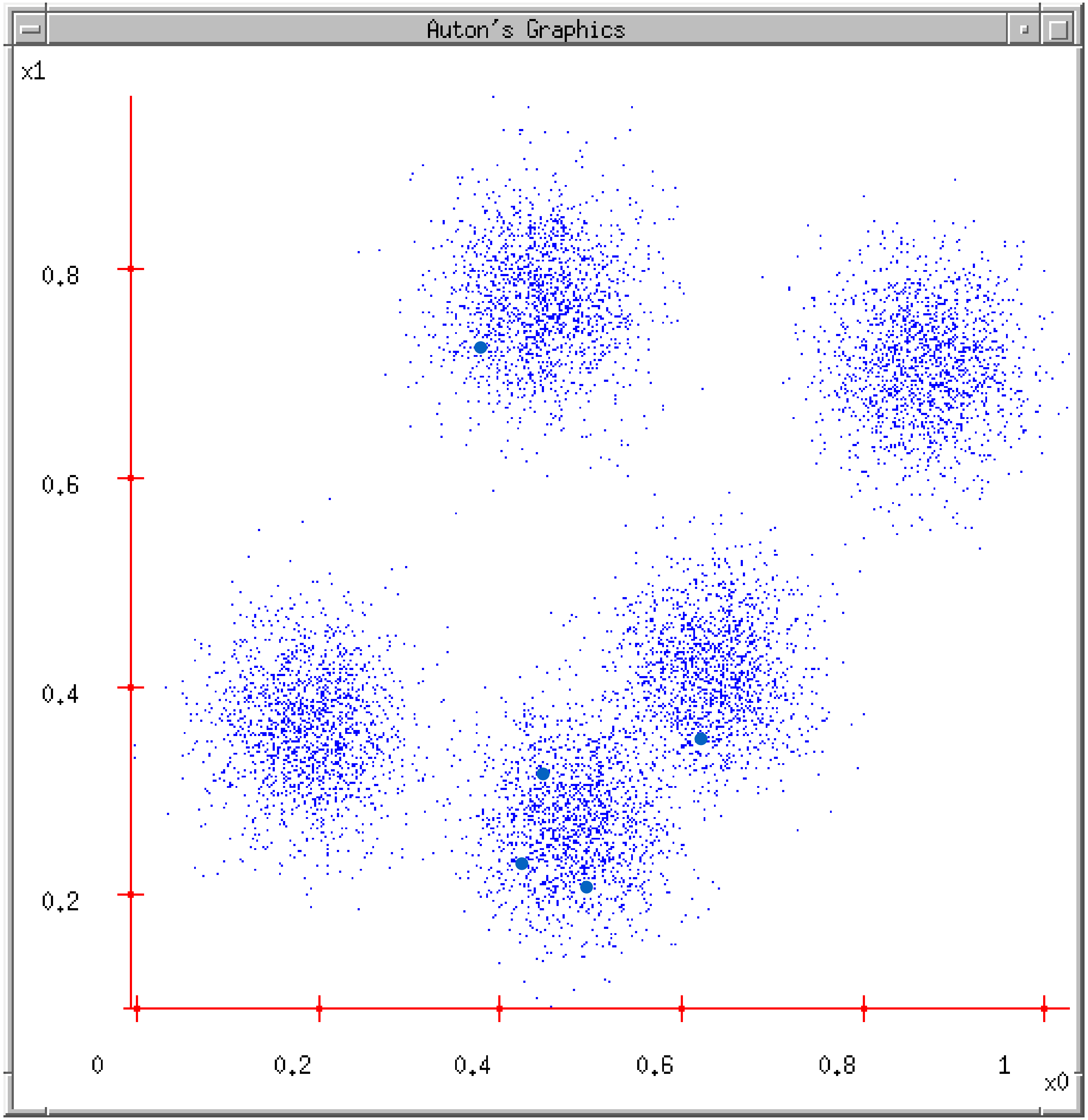
K-means

1. Ask user how many clusters they'd like. *(e.g. k=5)*
2. Randomly guess k cluster Center locations



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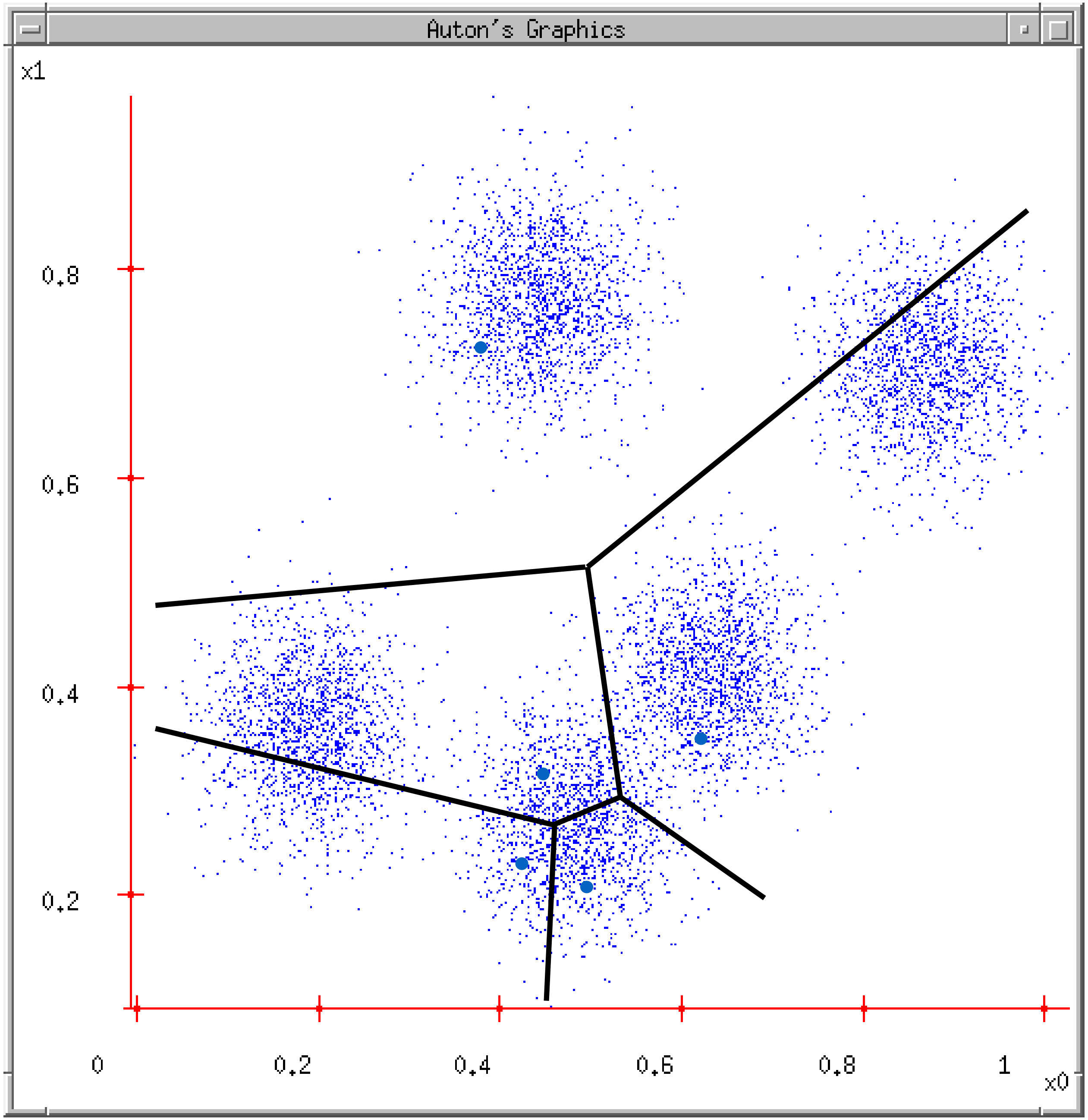
K-means

1. Ask user how many clusters they'd like. (e.g. k=5)
2. Randomly guess k cluster Center locations
3. Each datapoint finds out which Center it's closest to.



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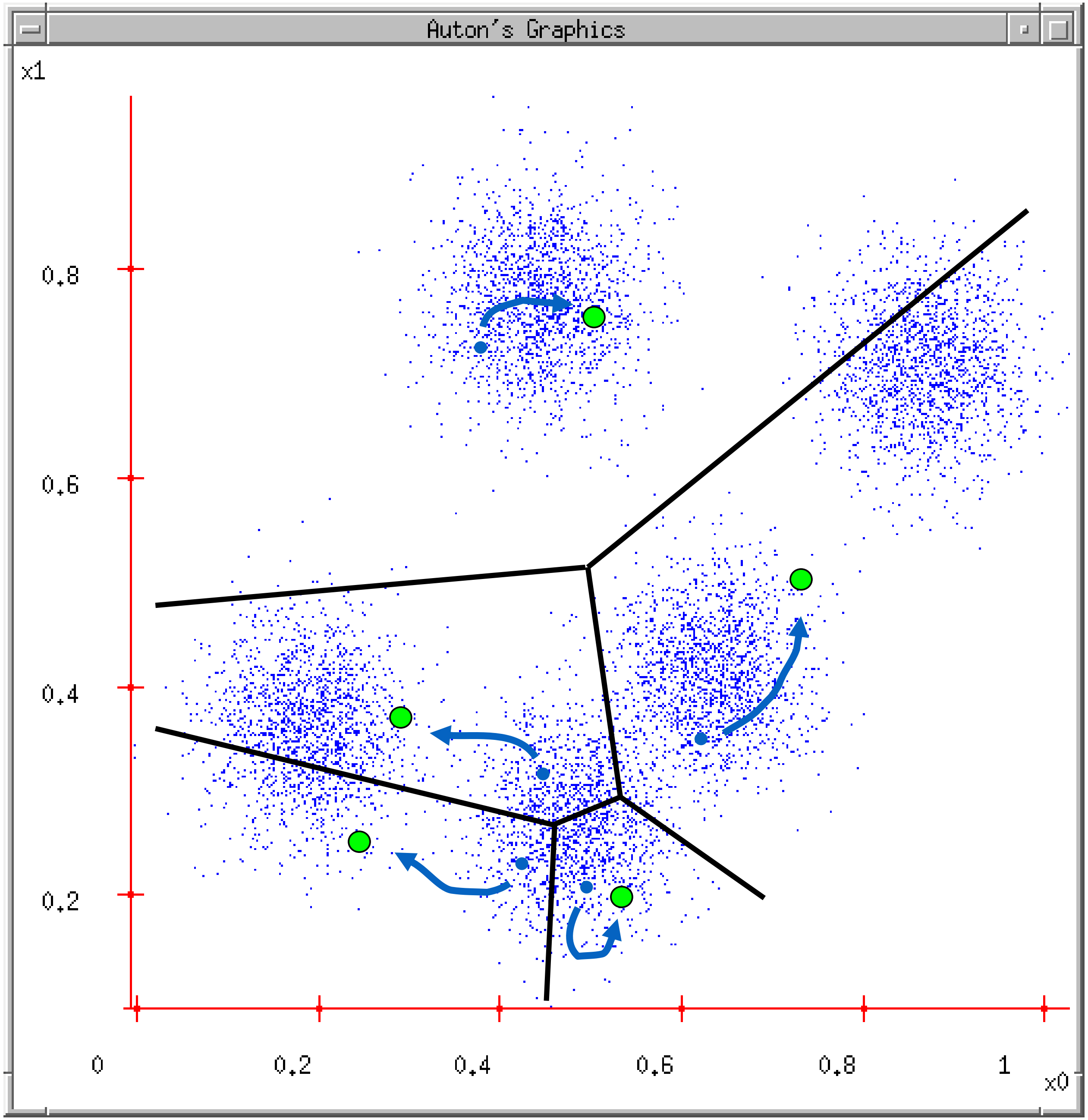
K-means

1. Ask user how many clusters they'd like. (e.g. k=5)
2. Randomly guess k cluster Center locations
3. Each datapoint finds out which Center it's closest to.
4. Each Center finds the centroid of the points it owns



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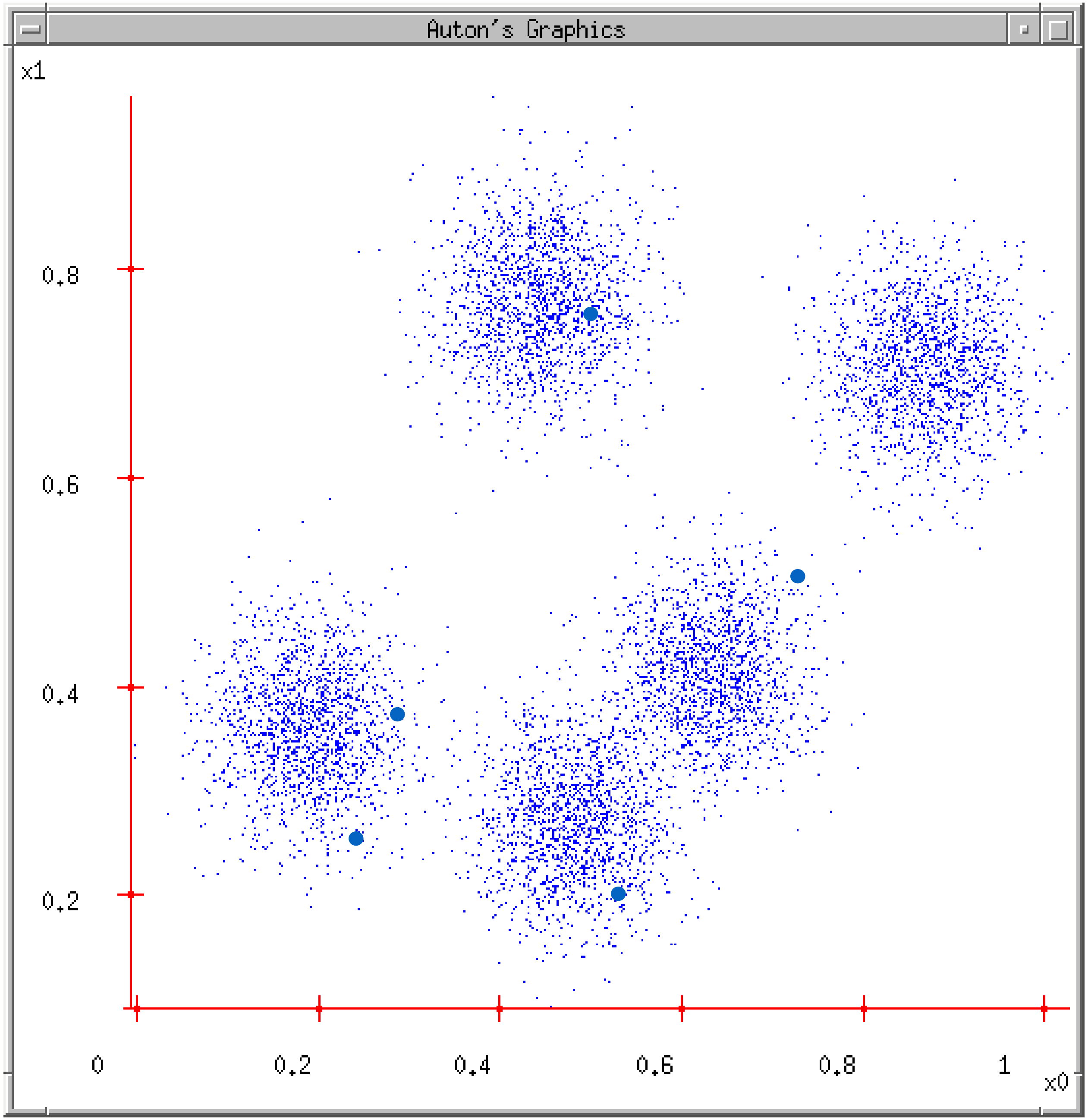
K-means

1. Ask user how many clusters they'd like. (e.g. k=5)
2. Randomly guess k cluster Center locations
3. Each datapoint finds out which Center it's closest to.
4. Each Center finds the centroid of the points it owns…
5. …and jumps there
6. …Repeat until terminated!



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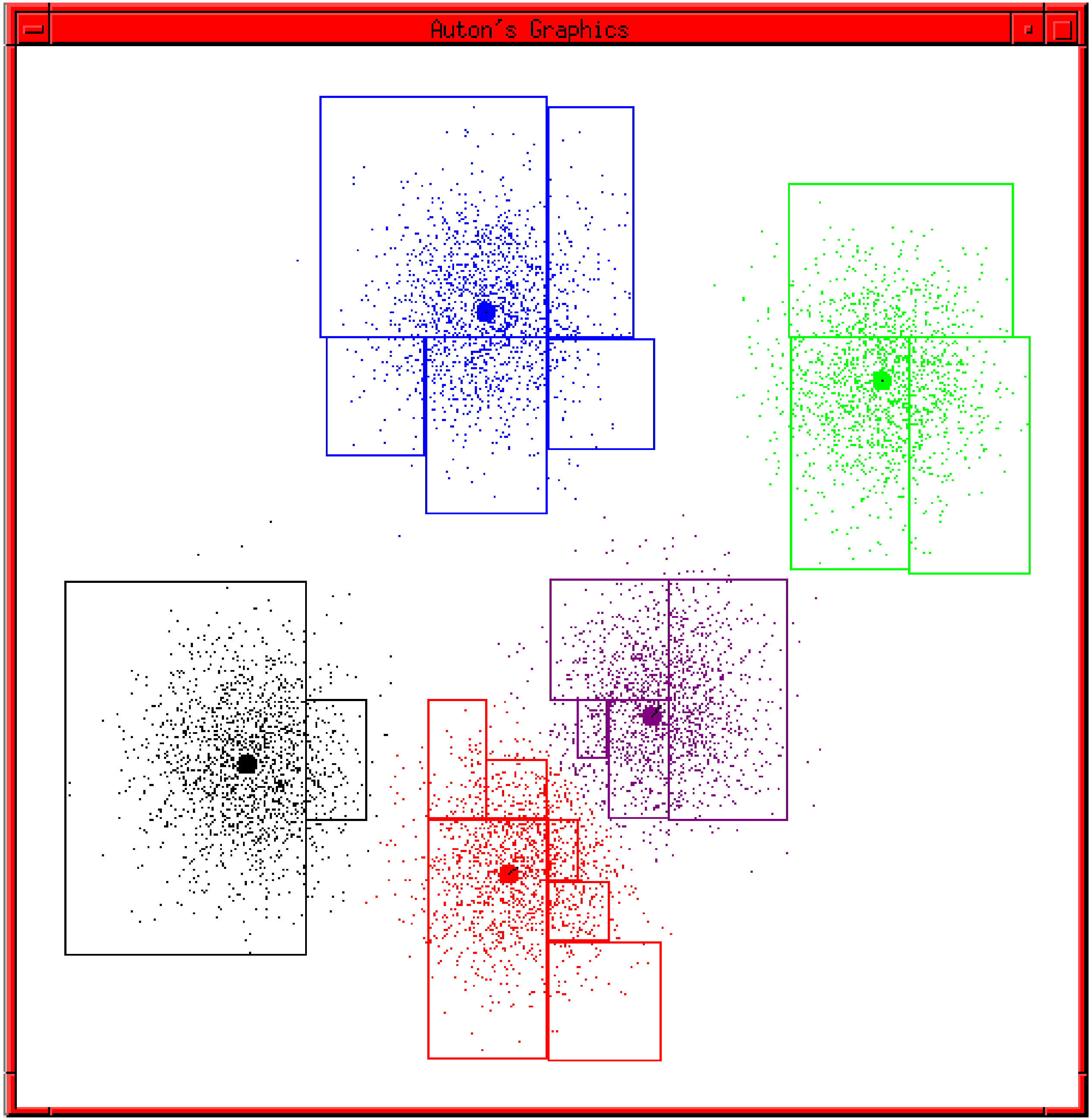
K-means

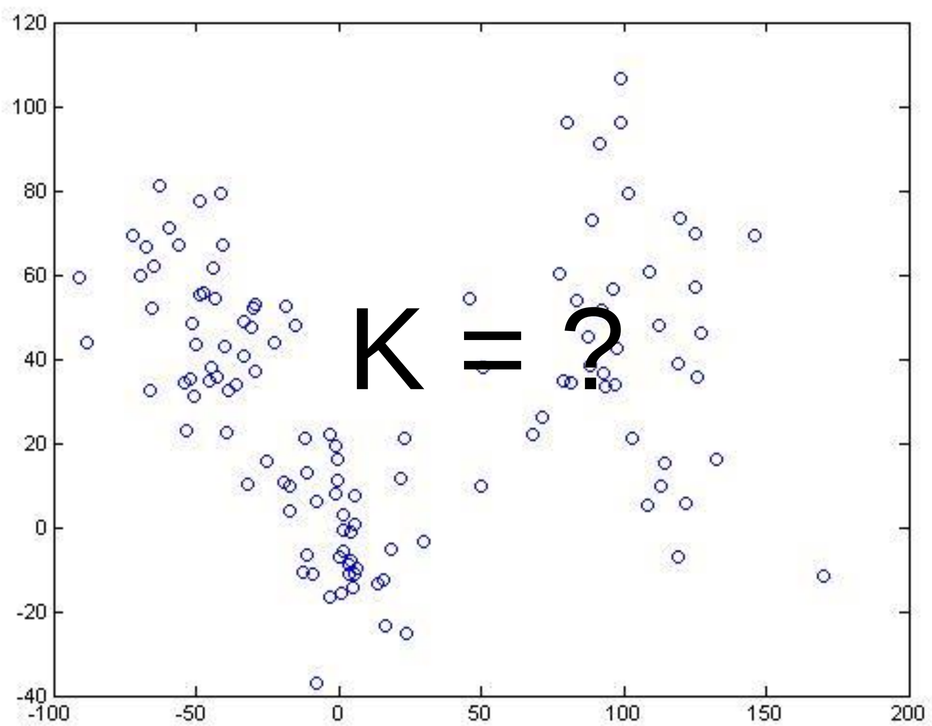


Example generated by Dan Pelleg's super-duper fast K-means system:

Dan Pelleg and Andrew Moore. Accelerating Exact k-means Algorithms with Geometric Reasoning. Proc. Conference on Knowledge Discovery in Databases 1999, (KDD99) (available on www.autonlab.org/pap.html*)*

https://reurl.cc/b779v

K-means Clustering Issues



How many clusters do you think there are in this data? How might it have been generated?

$$K \approx \sqrt{n/2}$$

Determining K

- We'd like to have a measure of cluster quality *Q* and then try different values of *k* until we get an optimal value for *Q*
- This is an unsupervised learning method; we can't really find a "correct" measure *Q*…

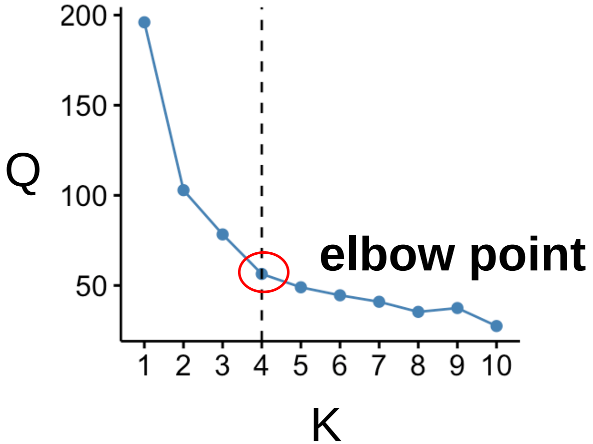
Cluster Quality Measures

- A measure that emphasizes cluster tightness or homogeneity:

$$Q = \sum_{i=1}^{k} \frac{1}{|C_i|} \sum_{\boldsymbol{x} \in C_i} d(\boldsymbol{x}, \mu_i)$$

Similar to Ward's Method!

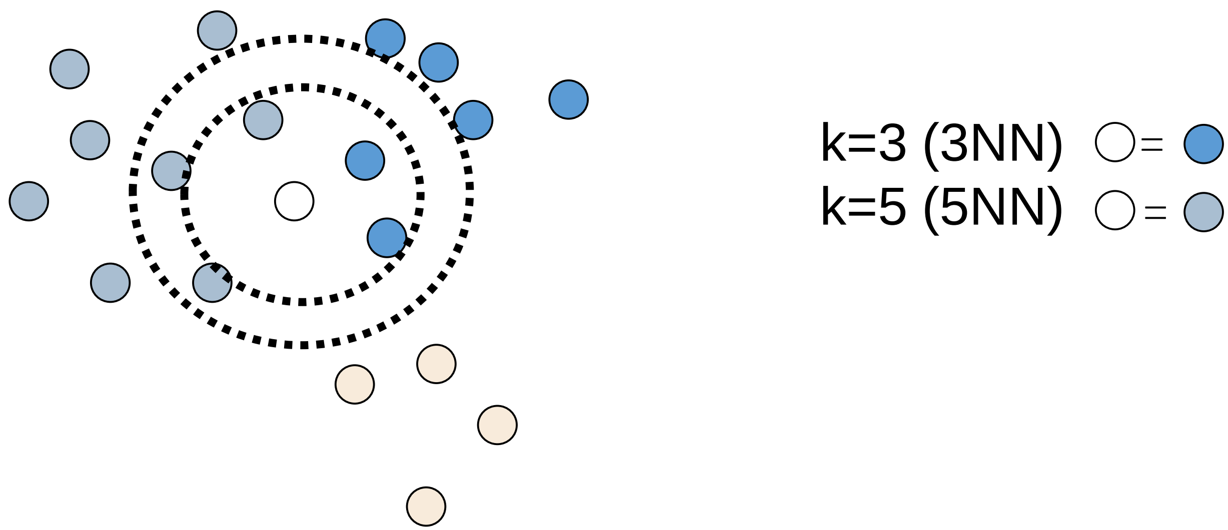
- $|C_i|$ is the number of data points in cluster *i*
- *Q* will be small if the data points in each cluster are close



- Don’t be confused by K-means and KNN

k-Nearest Neighbor (kNN)

- A supervised learning classifier



Summary

- Clustering is a very popular method of biomedical (e.g., microarray) analysis.
- Many variations on *k*-means, including algorithms in which clusters can be split and merged.
- Clustering algorithm can be used for classification. How?

https://colab.research.google.com/github/jakevdp/PythonDataScienceHandbook/blob/master/notebooks/05.11-K-Means.ipynb

Questions?

Did you finish your prohject?