Introduction to Data Science

GIRI NARASIMHAN, SCIS, FIU

Clustering

Clustering dogs using height & weight

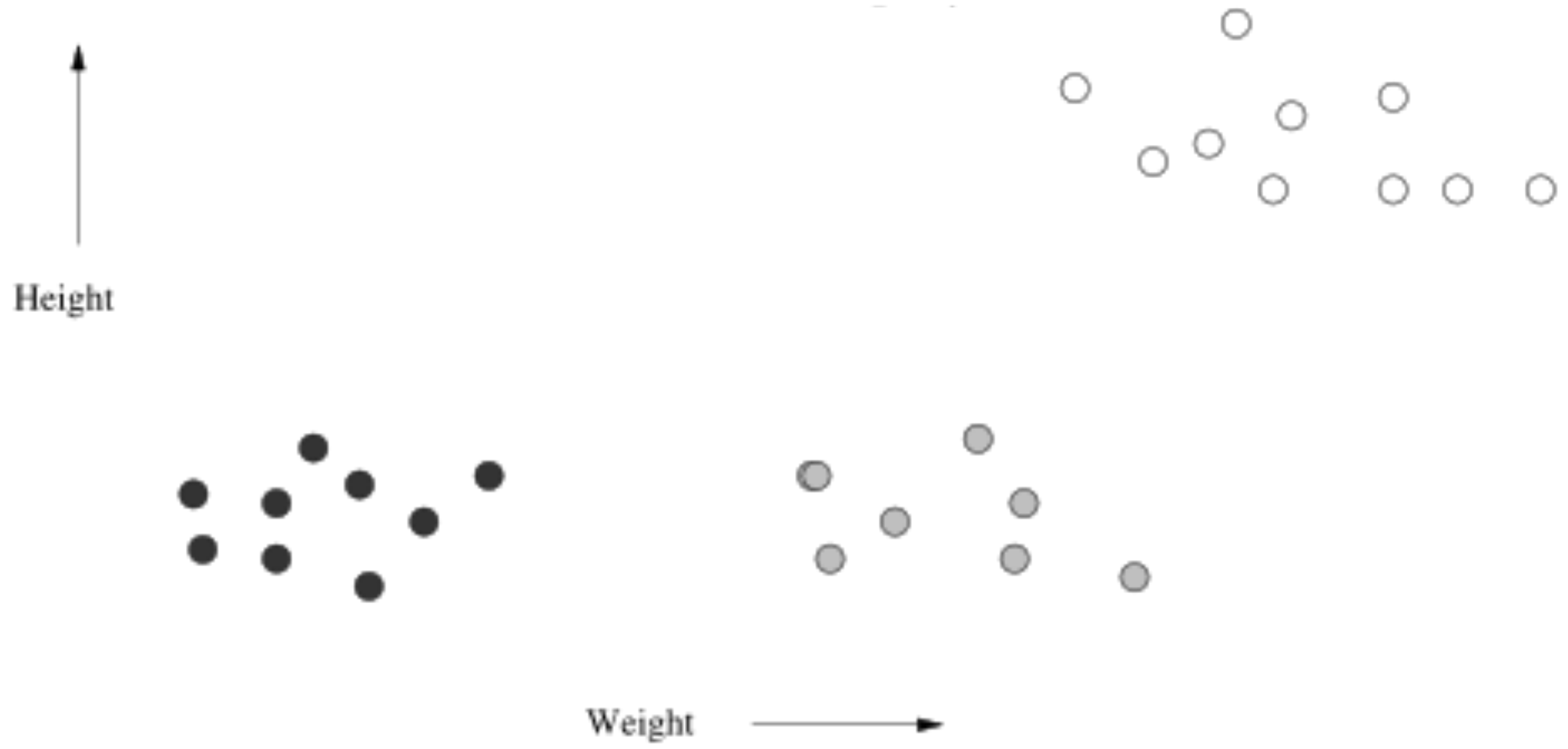


Figure 7.1: Heights and weights of dogs taken from three varieties

Clustering dogs using height & weight

Figure 7.1: Heights and weights of dogs taken from three varieties

Clustering

- Clustering is the process of making clusters, which put **similar** things together into same cluster …
- And put **dissimilar** things into different clusters
- Need a similarity function
- Need a ~~similarity~~ **distance** function
  - Convenient to map items to points in space

Distance Functions

- Jaccard Distance
- Hamming Distance
- Euclidean Distance
- Cosine Distance
- Edit Distance
- …

- What is a **distance** function
  - D(x,y) >= 0
  - D(x,y) = D(y,x)
  - D(x,y) <= D(x,z) + D(z,y)

Clustering Strategies

- Hierarchical or Agglomerative
  - Bottom-up
- Partitioning methods
  - Top-down
- Density-based
- Cluster-based
- Iterative methods

Curse of Dimensionality

- N points in d-dimensional unit (hyper)sphere
  - If d = 1, then average distance = 1/3
  - As d gets larger, what is the average distance? Distribution of distances?
    - # of **nearby** points for any given point **vanishes.** So, clustering does not work well
    - # of points at max distance (~sqrt(d)) also vanishes. Real range actually very small
  - Angle ABC given 3 points approaches 90
    - Denominator grows linearly with d
    - Expected cos = 0 since equal points expected in all 4 quadrants

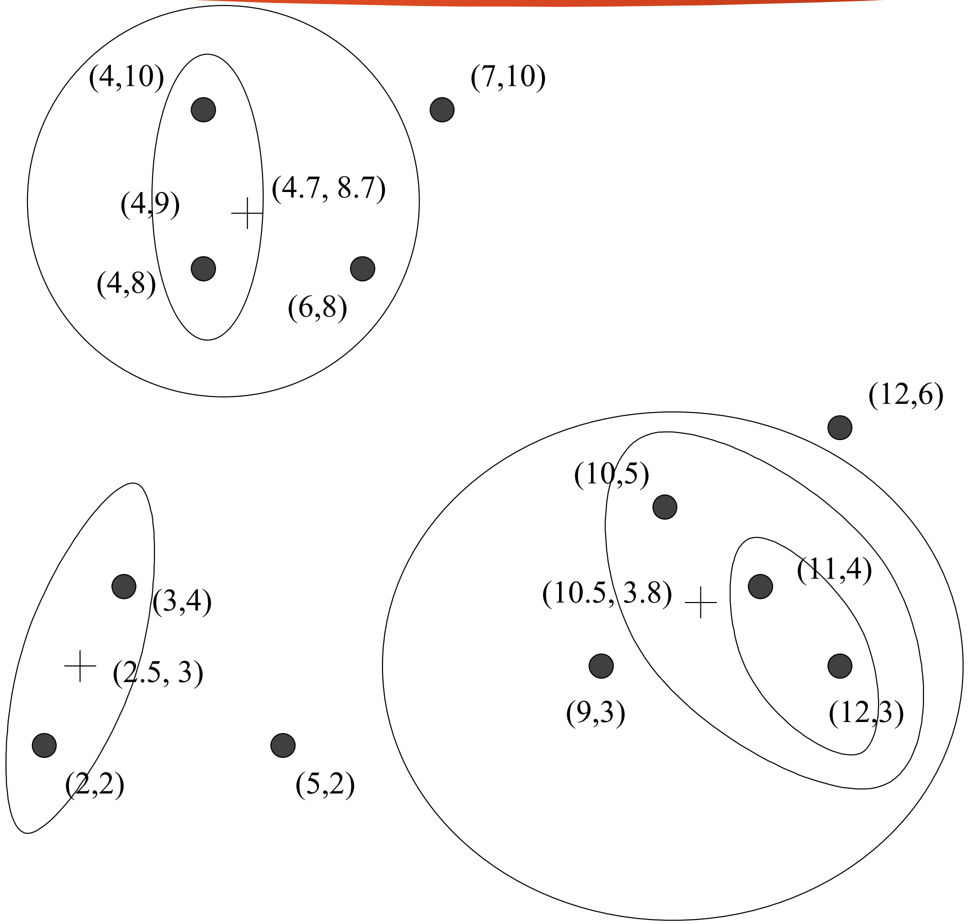
$$\frac{\sum_{i=1}^{d} x_i y_i}{\sqrt{\sum_{i=1}^{d} x_i^2}\sqrt{\sum_{i=1}^{d} y_i^2}}$$

Hierarchical Clustering

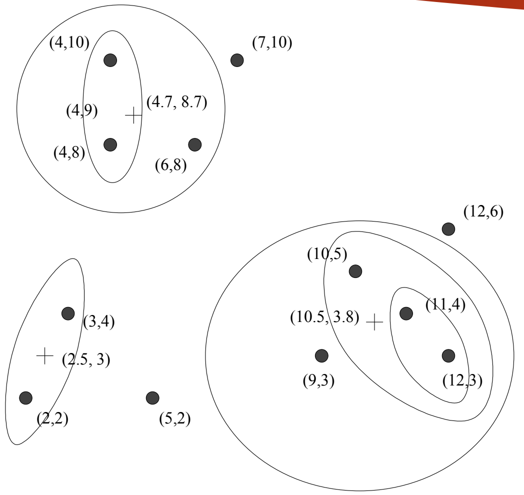
Hierarchical Clustering

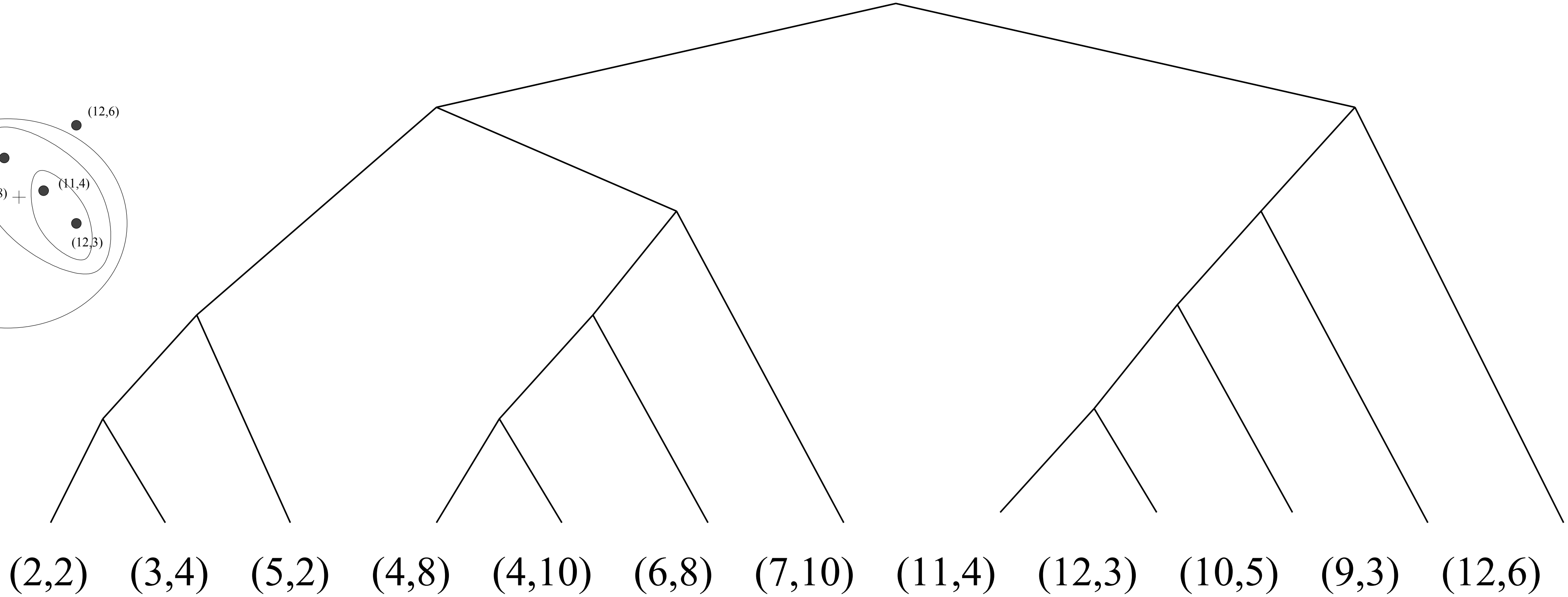
- Starts with each item in different clusters
- Bottom up
- In each iteration
  - Two clusters are identified and merged into one
- Items are combined as the algorithm progresses
- **Questions**:
  - How are clusters represented
  - How to decide which ones to merge
  - What is the sopping condition
- Typical algorithm: find smallest distance between nodes of different clusters

Hierarchical Clustering



Output of Clustering: Dendrogram





Measures for a cluster

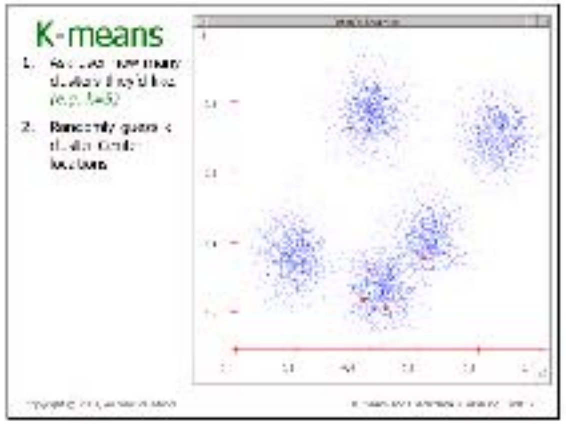
- Radius: largest distance from a centroid
- Diameter: largest distance between some pair of points in cluster
- Density: # of points per unit volume
- Volume: some power of radius or diameter
- Tightness, separation, …
- **Good cluster**: when diameter of each cluster is much larger than its nearest cluster or nearest point outside cluster

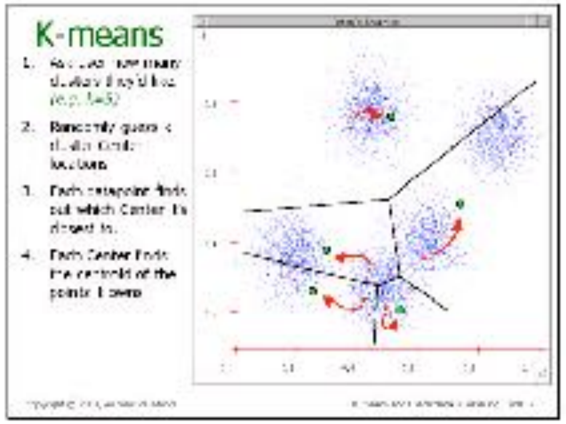
Stopping condition for clustering

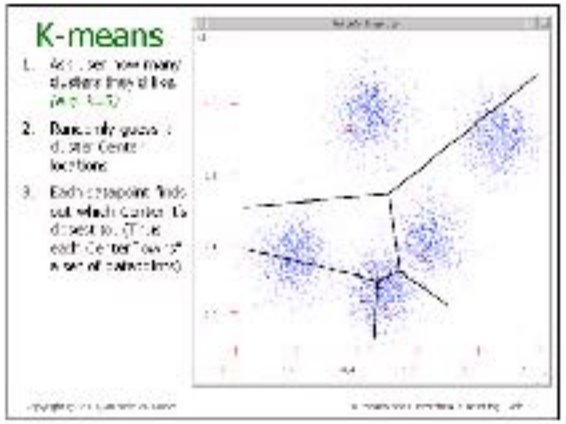
- Cluster radius or diameter crosses a threshold
- Cluster density drops below a certain threshold
- Ratio of diameter to distance to nearest cluster drops below a certain threshold

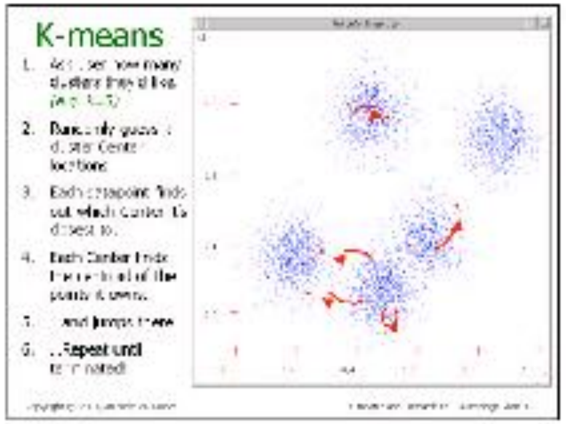
K-Means Clustering

Start









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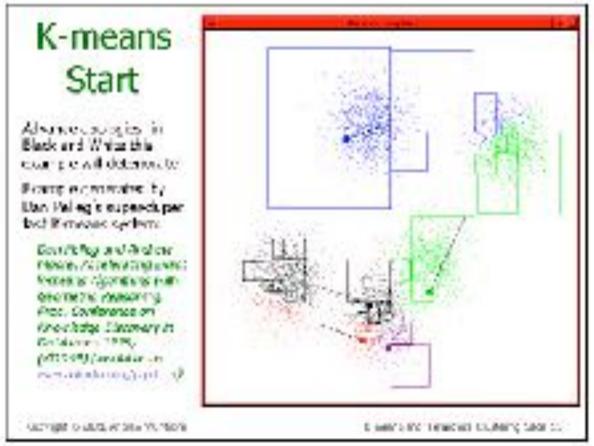
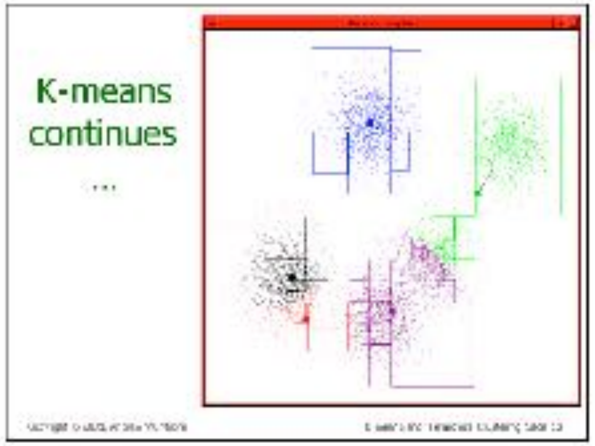
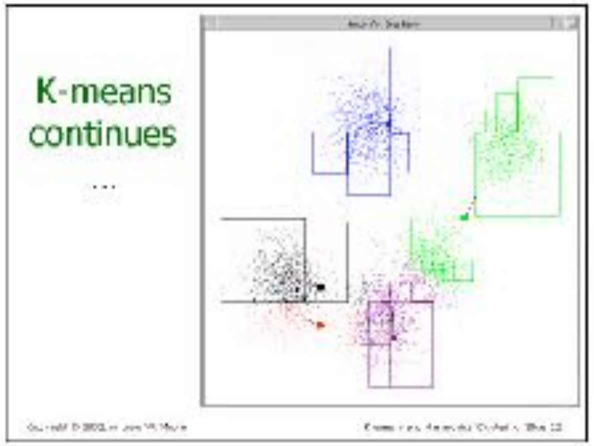
Example from Andrew Moore's tutorial on Clustering.







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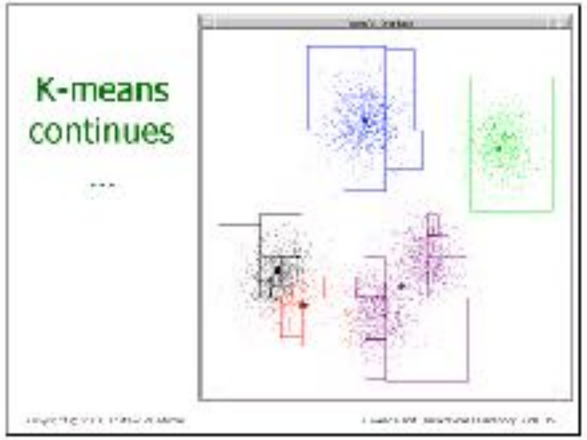

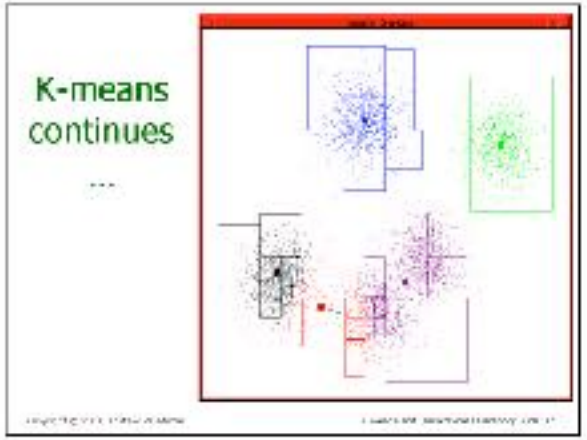

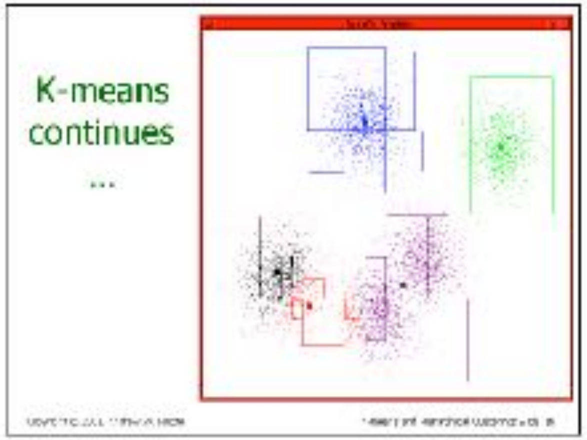

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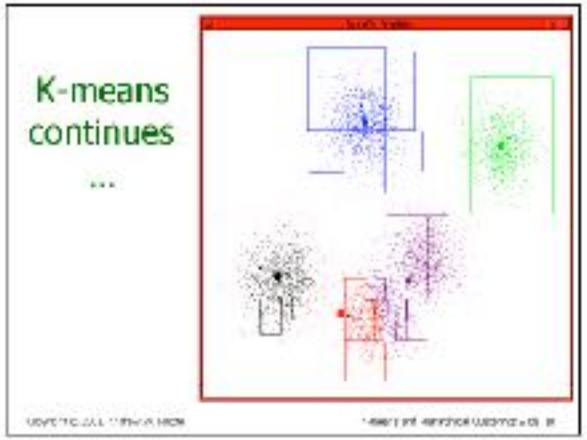

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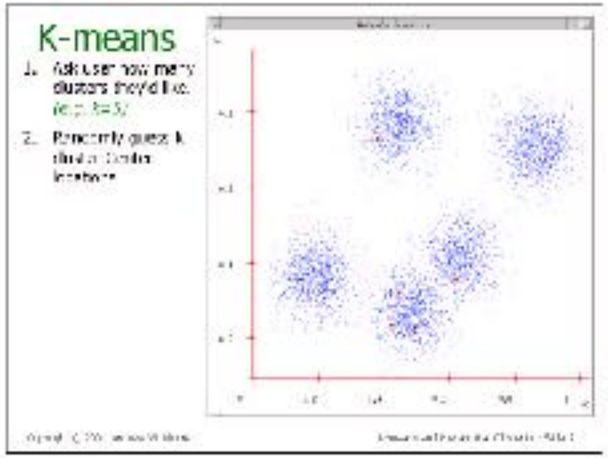
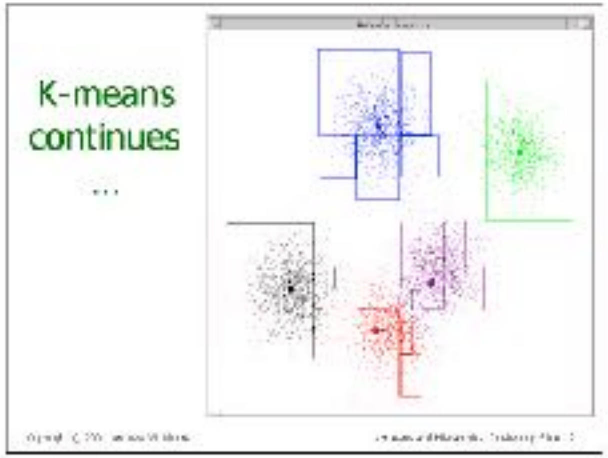
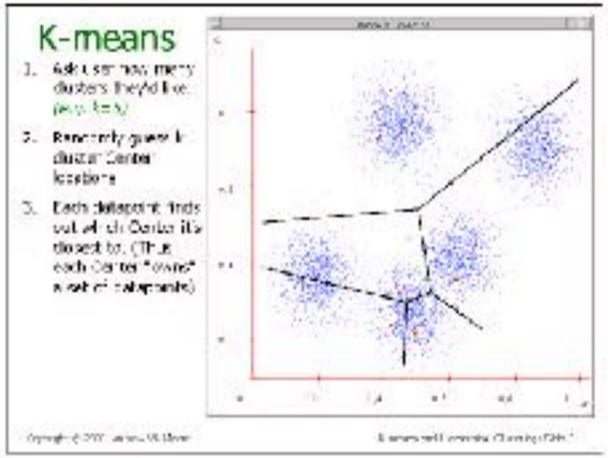
Example from Andrew Moore's tutorial on Clustering.

Start







End

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Example from Andrew Moore's tutorial on Clustering.

K-Means Clustering [McQueen '67]

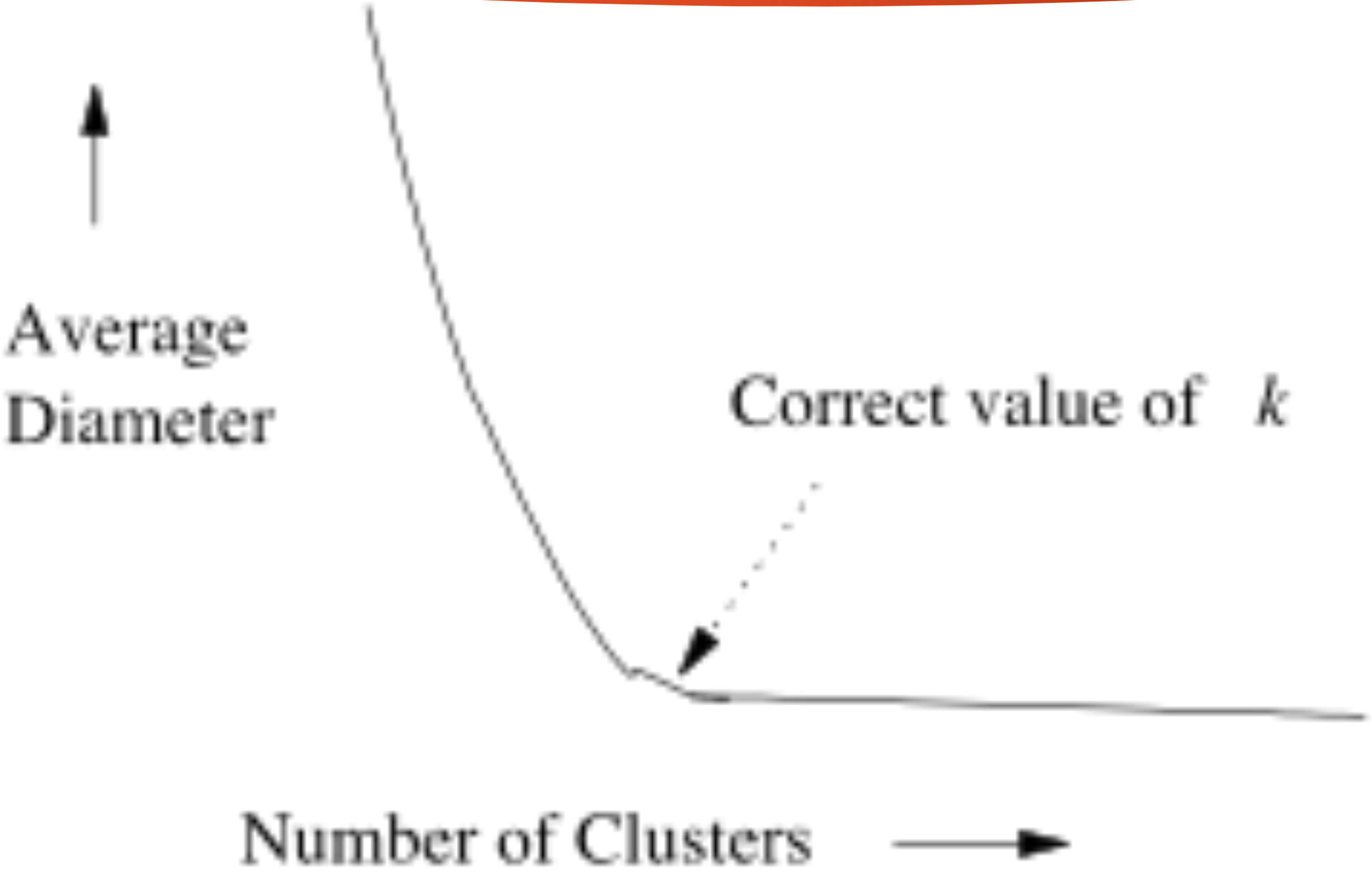
Repeat

- Start with randomly chosen cluster centers
- Assign points to give greatest increase in score
- Recompute cluster centers
- Reassign points

until (no changes)

Try the applet at: http://home.dei.polimi.it/matteucc/Clustering/tutorial_html/AppletH.html

How to find K for K-means?



Comparisons

- Hierarchical clustering
  - Number of clusters not preset.
  - Complete hierarchy of clusters
  - Not very robust, not very efficient.
- K-Means
  - Need definition of a mean. Categorical data?
  - Can be sensitive to initial cluster centers; Stopping condition unclear
  - More efficient and often finds optimum clustering.

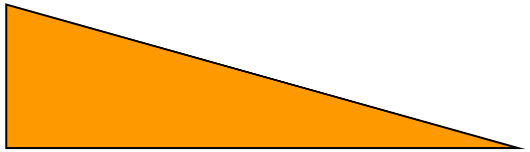
Implementing Clustering

Example High-Dim Application: SkyCat

- A catalog of 2 billion "sky objects" represents objects by their radiation in 7 dimensions (frequency bands).
- Problem: cluster into similar objects, e.g., galaxies, nearby stars, quasars, etc.
- Sloan Sky Survey is a newer, better version.

Curse of Dimensionality

- Assume random points within a bounding box, e.g., values between 0 and 1 in each dimension.
- In 2 dimensions: a variety of distances between 0 and 1.41.
- In 10,000 dimensions, the difference in any one dimension is distributed as a triangle.



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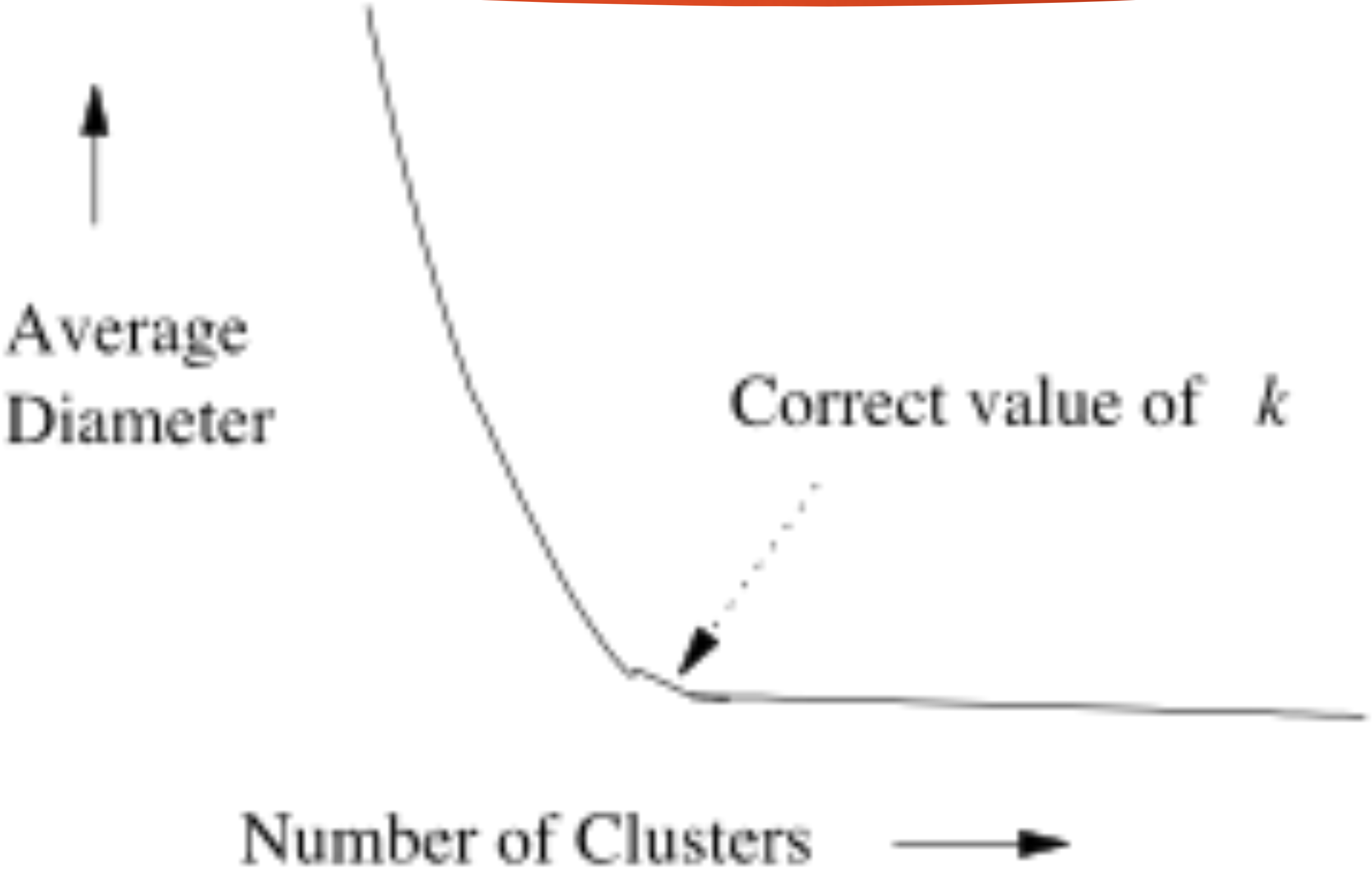


BFR Algorithm

- BFR (Bradley-Fayyad-Reina) – variant of *K* -means for very large (disk-resident) data sets.
- Assumes that clusters are normally distributed around a centroid in Euclidean space.
  - SDs in different dimensions may vary

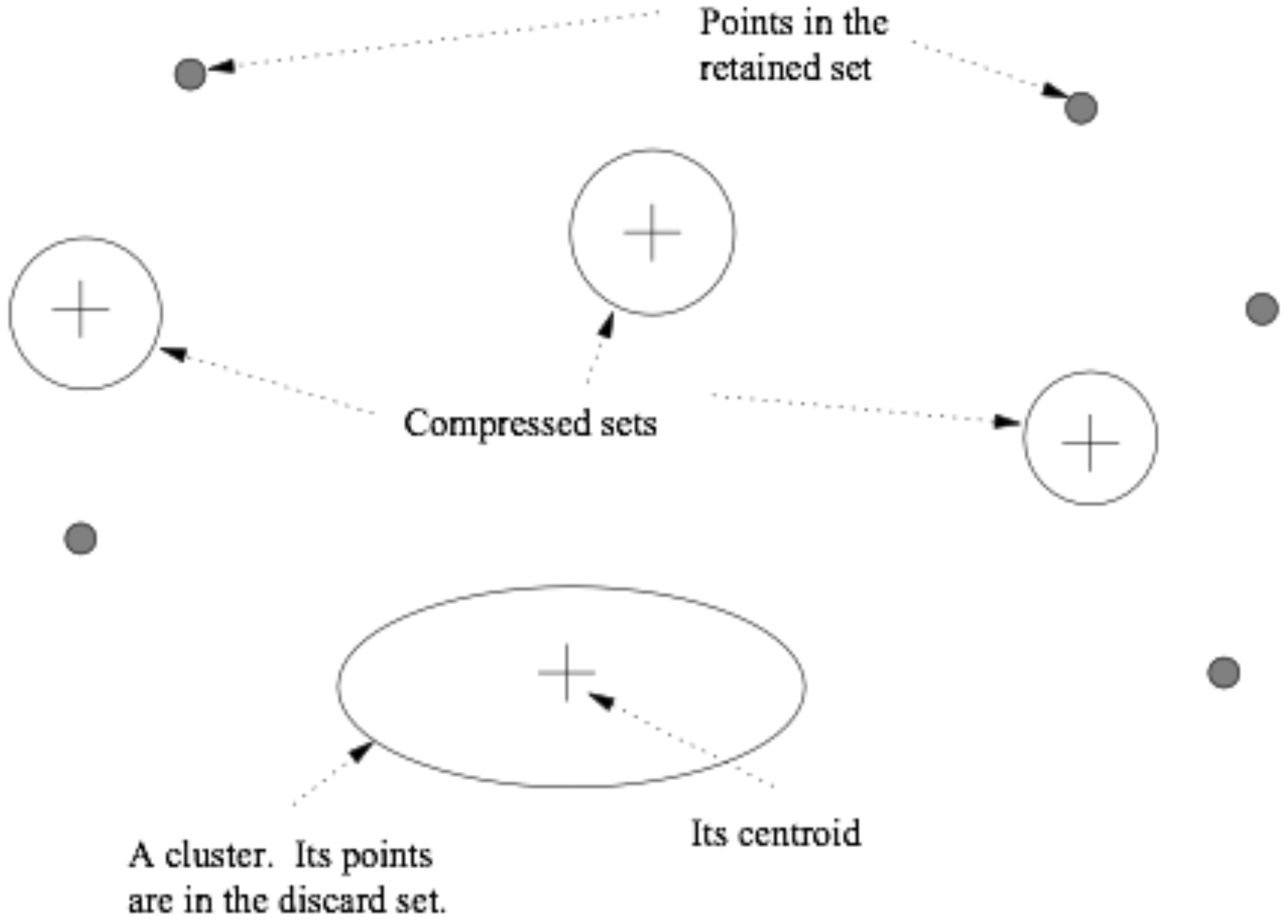
BFR … 2

- Points read "chunk" at a time.
- Most points from previous chunks summarized by simple statistics.
- First load handled by some sensible approach:
  1. Take small random sample and cluster optimally.
  2. Take sample; pick random point, & $k - 1$ more points incrementally, each as far from previously points as possible.

BFR … 3

1. *Discard set* : points close enough to a centroid to be summarized.
2. *Compression set* : groups of points that are close together but not close to any centroid. They are summarized, but not assigned to a cluster.
3. *Retained set* : isolated points.

BFR … 4


Points in the
retained set
Compressed sets
A cluster. Its points
are in the discard set.
Its centroid

BFR: How to summarize?

- Discard Set & Compression Set: N, SUM, SUMSQ
- 2d + 1 values
- Average easy to compute
  - SUM/N
- SD not too hard to compute
  - VARIANCE = (SUMSQ/N) – $(SUM/N)^2$

BFR: Processing

- Maintain N, SUM, SUMSQ for clusters
- Policies for merging compressed sets needed and for merging a point in a cluster
- Last chunk handled differently
  - Merge all compressed sets
  - Merge all retained sets into nearest clusters
- BFR suggests **Mahalanobis Distance**

Mahalanobis Distance

- Normalized Euclidean distance from centroid.
- For point $(x_1,\ldots,x_k)$ and centroid $(c_1,\ldots,c_k)$:

1. Normalize in each dimension: $y_i = (x_i - c_i)/\sigma_i$
2. Take sum of the squares of the y_i's.
3. Take the square root.

- For Gaussian clusters, ~65% of points within SD dist

GRPGF Algorithm

GRPGF Algorithm

- Works for non-Euclidean distances
- Efficient, but approximate
- Works well for high dimensional data
  - Exploits orthogonality property for high dim data
- Rules for splitting and merging clusters

Clustering for Streams

- BDMO (authors, B. Babcock, M. Datar, R. Motwani, & L. O'Callaghan)
- Points of stream partitioned into, and summarized by, buckets with sizes equal to powers of two. Size of bucket is number of points it represents.
- Sizes of buckets obey restriction that <= two of each size. Sizes are required to form a sequence -- each size twice previous size, e.g., 3,6,12,24,... .
- Bucket sizes restrained to be nondecreasing as we go back in time. As in Section 4.6, we can conclude that there will be O(log N) buckets.
- Rules for initializing, merging and splitting buckets