Unsupervised Learning with Clustering

K-means EM clustering Hierarchical Clustering





Why Clustering

- A good grouping implies some structure
- In other words, given a good grouping, we can then:
 - Interpret and label clusters
 - Identify important features
 - Characterize new points by the closest cluster (or nearest neighbors)
 - Use the cluster assignments as a compression or summary of the data





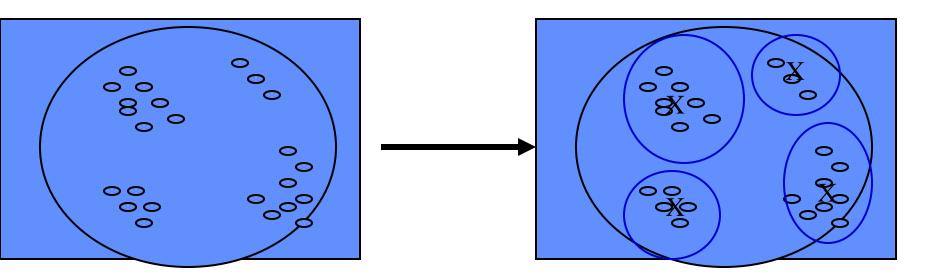
Clustering

- Basic idea: Group similar things together
- Unsupervised Learning Useful when no other info is available
- K-means
 - Partitioning instances into k disjoint clusters
 - Measure of similarity





Clustering







Clustering Techniques

- K-means clustering
- Hierarchical clustering
- Conceptual clustering
- Probability-based clustering
- Bayesian clustering





Clustering Techniques

- K-means clustering
- Hierarchical clustering
- Conceptual clustering
- Probability-based clustering
- Bayesian clustering





Clustering Applications

- Example: Clustering of a large number of gene experiments
- Multiple sequence alignment of genes closely clustered together
- Search for metabolic pathways genes may be involved with
- Possible functional classification of genes in the same cluster
- Identifying co-regulated genes from expression arrays





Common uses of Clustering

- Often used as an exploratory data analysis tool
- In one-dimension, a good way to quantify realvalued variables into k non-uniform buckets
- Used on acoustic data in speech understanding to convert waveforms into one of k categories (known as Vector Quantization)
- Also used for choosing color palettes on old fashioned graphical display devices
- Color Image Segmentation





Clustering

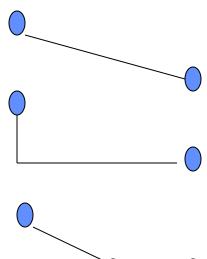
- Unsupervised: no target value to be predicted
- Differences ways clustering results can be produced/represented/learned
 - Exclusive vs. overlapping
 - Deterministic vs. probabilistic
 - Hierarchical vs. flat
 - Incremental vs. batch learning

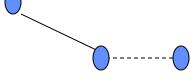




Clustering Objective

- Objective: find subsets that are similar within cluster and dissimilar between clusters
- Similarity defined by distance measures
 - Fuclidean distance
 - Manhattan distance
 - Mahalanobis (Euclidean w/dimensions rescaled by variance)





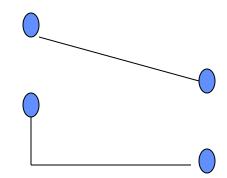


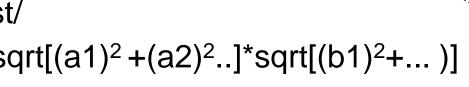


Clustering Objective

- Objective: find subsets that are similar within cluster and dissimilar between clusters
- Similarity defined by distance measures
 - Euclidean distance = $sqrt[(a1 - b1)^2 + (a2 - b2)^2 + ...)]$
 - Manhattan distance [|a1 - b1| + |a2 - b2| + ...)]
 - Cosine (insensitive to size) **Euc Dist/**

$$sqrt[(a1)^2+(a2)^2..]*sqrt[(b1)^2+...)]$$









The k-means Algorithm Iterative Distance Based Clustering

- Clusters the data into k groups where k is specified in advance
 - 1. Cluster centers are chosen at random
 - 2. Instances are assigned to clusters based on their distance to the cluster centers
 - 3. Centroids of clusters are computed "means"
 - 4. Go to 1st step until convergence





K-means Clustering

A simple, effective, and standard method

Start with K initial cluster centers

Loop:

Assign each data point to nearest cluster center Calculate mean of cluster for new center Stop when assignments don't change

Issues:

How to choose K?

How to choose initial centers?

Will it always stop?





K-Means Clustering Pros & Cons

- Simple and reasonably effective
- The final cluster centers do not represent a global minimum but only a local one
- Result can vary significantly based on initial choice of seeds
 - Completely different final clusters can arise from differences in the initial randomly chosen cluster centers
- Algorithm can easily fail to find a reasonable clustering





Getting Trapped in a Local Minimum

- Example: four instances at the vertices of a twodimensional rectangle
 - Local minimum: two cluster centers at the midpoints of the rectangle's long sides

 Simple way to increase chance of finding a global optimum: restart with different random seeds





Clustering

- Partition unlabeled examples into disjoint subsets of clusters, such that:
 - Examples within a cluster are very similar
 - Examples in different clusters are very different
- Discover new categories in an unsupervised manner (no sample category labels provided)





K-Means Algorithm

Let d be the distance measure between instances.

Select k random instances $\{s_1, s_2, \dots s_k\}$ as seeds.

Until clustering converges or other stopping criterion:

For each instance x_i :

Assign x_i to the cluster c_j such that $d(x_i, s_j)$ is minimal.

(Update the seeds to the centroid of each cluster)

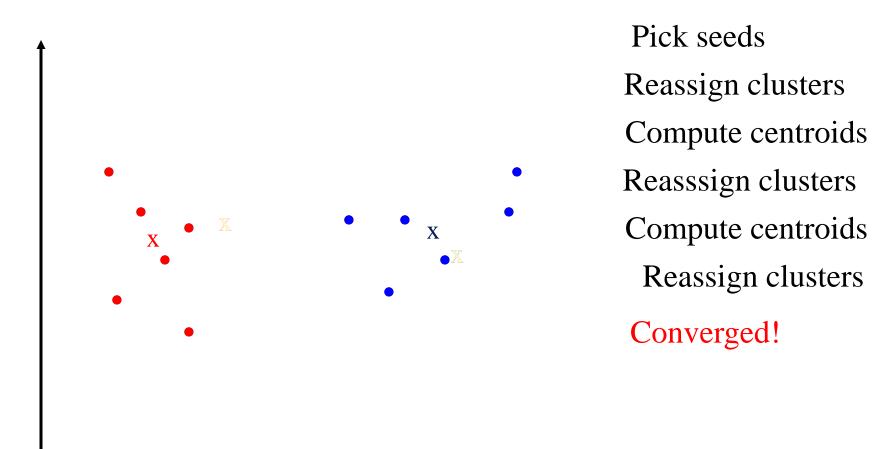
For each cluster c_j

$$s_j = \mu(c_j)$$





K Means Example (K=2)



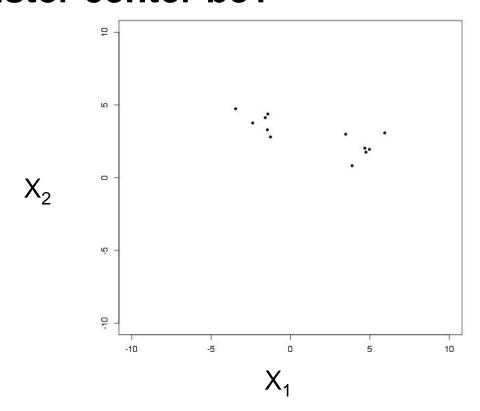
Seed Choice

- Results can vary based on random seed selection
- Some seeds can result in poor convergence rate, or convergence to sub-optimal clusters
- Select good seeds using a heuristic or the results of another method





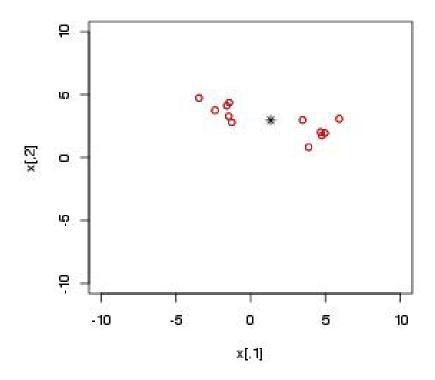
 For K=1, using Euclidean distance, where will the cluster center be?







 For K=1, the overall mean minimizes Sum Squared Error (SSE), aka Euclidean distance



Simple example:

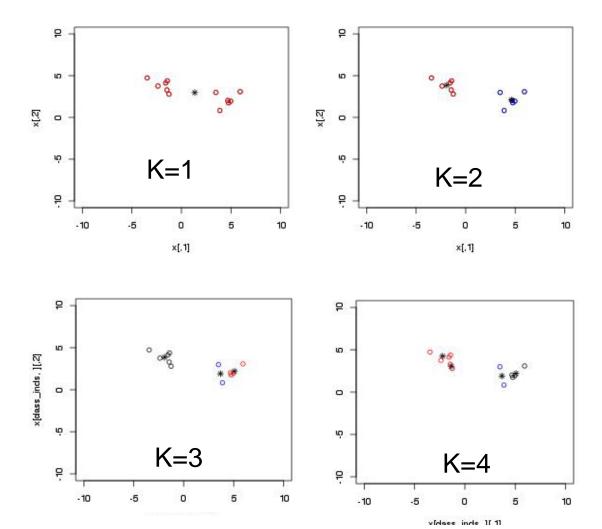
#choose 1 data point as initial K centers

#10 is max loop iterations

#1 is number of initial sets to try

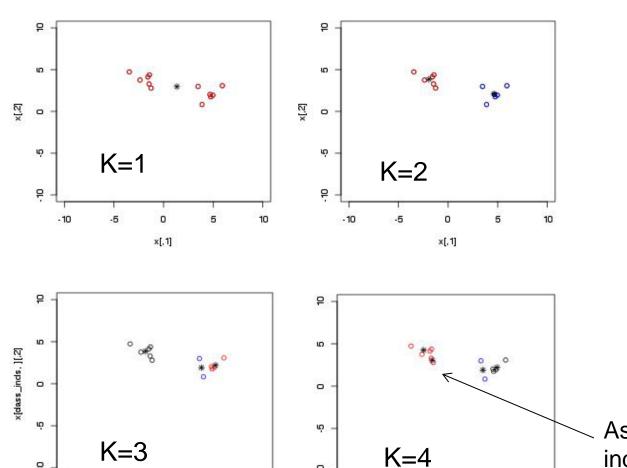


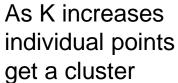














무



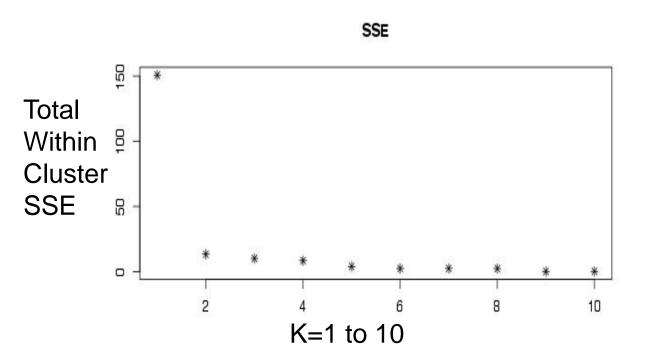
무

-10

-5

vidace inde 11 11

Choosing K for K-means



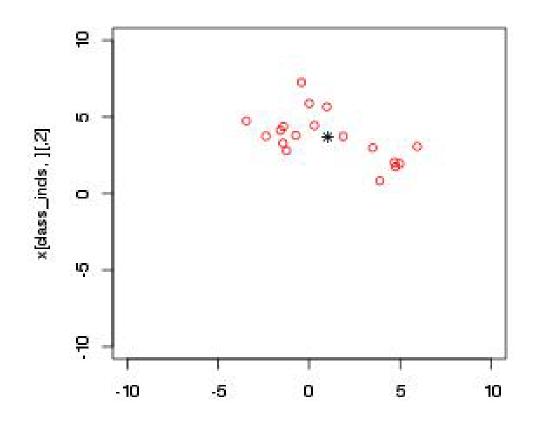
- Not much improvement after K=2 ("elbow")





K-means Example – more points

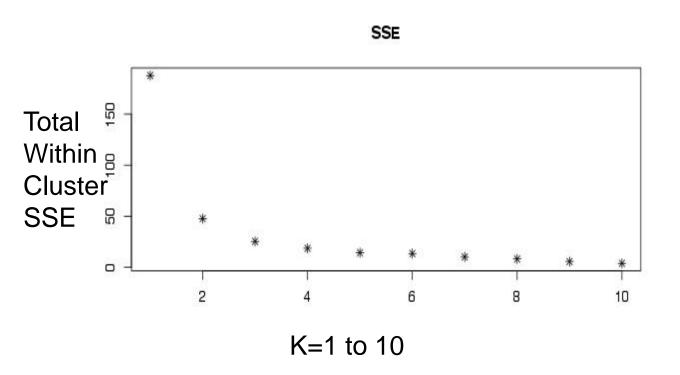
How many clusters should there be?







Choosing K for K-means



- Smooth decrease at K ≥ 2, harder to choose
- In general, smoother decrease => less structure





K-means Guidelines

Choosing K:

- "Elbow" in total-within-cluster SSE as K=1...N
- Cross-validation: hold out points, compare fit as K=1...N

Choosing initial starting points:

 take K random data points, do several K-means, take best fit

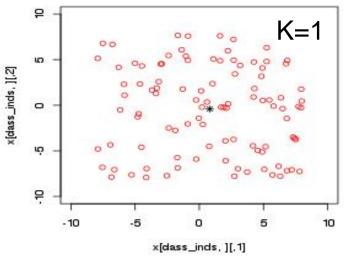
Stopping:

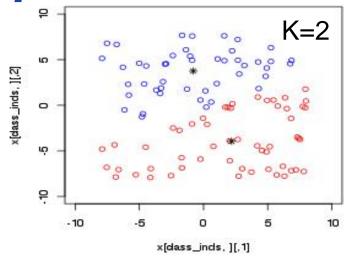
- may converge to sub-optimal clusters
- may get stuck or have slow convergence (point assignments bounce around), 10 iterations is often good

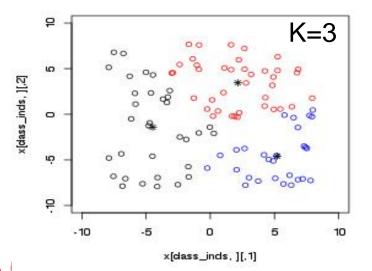


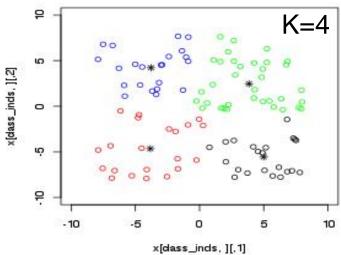


K-means Example: uniform dist.





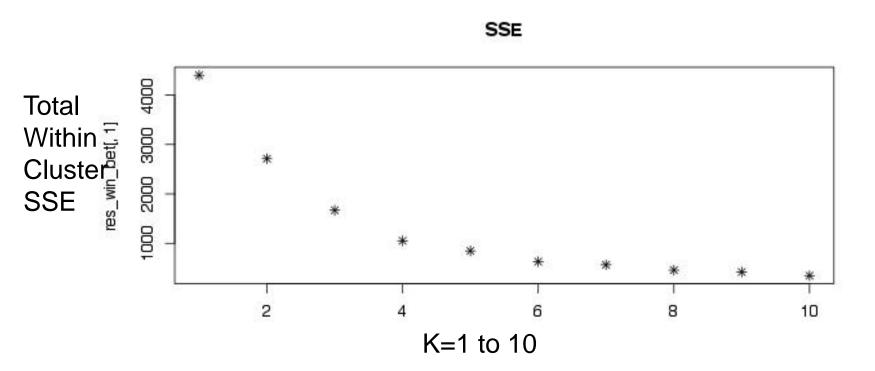






Predictive Analytics Center of Excellence

Choosing K - uniform



- Smooth decrease across K => less structure





K-means Clustering Issues

Scale:

Dimensions with large numbers may dominate distance metrics

Outliers:

Outliers can pull cluster mean, K-mediods uses median instead of mean





Probability-based Clustering

- Problems with K-means & Hierarchical methods:
 - Division by k
 - Order of examples
 - Merging/splitting operations might not be sufficient to reverse the effects of bad initial ordering
 - Is result at least local minimum of category utility?
- Solution:
 - Find the most likely clusters given the data
- Instance has certain probability of belonging to a particular cluster





Soft Clustering

- So far clustering methods assumed that each instance has a "hard" assignment to exactly one cluster
- No uncertainty about class membership or an instance belonging to more than one cluster
- Soft clustering gives probabilities that an instance belongs to each of a set of clusters
- Each instance is assigned a probability distribution across a set of discovered clusters
 - probabilities of all categories must sum to 1





Soft Clustering Methods

Fuzzy Clustering

- Use weighted assignments to all clusters
- Weights depend on relative distance
- Find min weighted SSE

Expectation-Maximization:

- Initialize a mixture of multivariate Gaussian distributions
- Find means, variances, and mixture weights that maximize probability of data





Finite mixtures

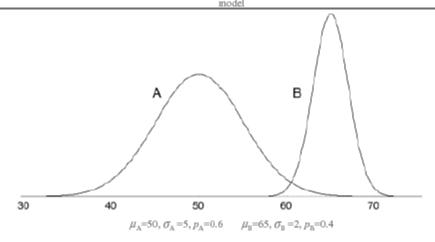
- Probabilistic clustering algorithms model the data using a mixture of distributions
- Each cluster is represented by one distribution
 - The distribution governs the probabilities of attributes values in the corresponding cluster
- They are called finite mixtures because there is only a finite number of clusters being represented
- Usually individual distributions are normal
- Distributions are combined using cluster weights





A Two-Class Mixture Model

						data					
A	51	В	62	В	64	A	48	A	39	A	51
A	43	A	47	A	51	В	64	В	62	A	48
В	62	A	52	A	52	A	51	В	64	В	64
В	64	В	64	В	62	В	63	A	52	A	42
A	45	A	. 51	A	49	A	43	В	63	A	48
A	42	В	65	A	48	В	65	В	64	A	41
A	46	A	48	В	62	В	66	A	48		
A	45	A	49	A	43	В	65	В	64		
A	45	A	46	A	40	A	46	A	48		
						1.1					







Using the Mixture Model

 The probability of an instance x belonging to cluster A is:

$$PR[A|x] = \frac{Pr[x|A]Pr[A]}{Pr[x]} = \frac{f(x; \mu_A, \sigma_A)p_A}{Pr[x]}$$





Learning the Clusters

- Assume we know that there are k clusters
- To learn the clusters we need to determine their parameters
 - I.e. their means and standard deviations
- Start with the initial guess for the 5
 parameters use them to calculate cluster
 probabilities for each instance, use these
 probabilities to re estimate the parameters
 and repeat
- We actually have a performance criterion: the likelihood of the training data given the clusters

Expectation Maximization (EM)

- Probabilistic method for soft clustering
- Iterative method for learning probabilistic categorization model from unsupervised data
- Direct method that assumes k clusters: $\{c_1, c_2, \dots c_k\}$
- Soft version of k-means
- Assumes a probabilistic model of categories that allows computing P(c_i | E) for each category, c_i, for a given example, E





EM Algorithm

- Initially assume random assignment of examples to categories
- Learn an initial probabilistic model by estimating model parameters from this randomly labeled data





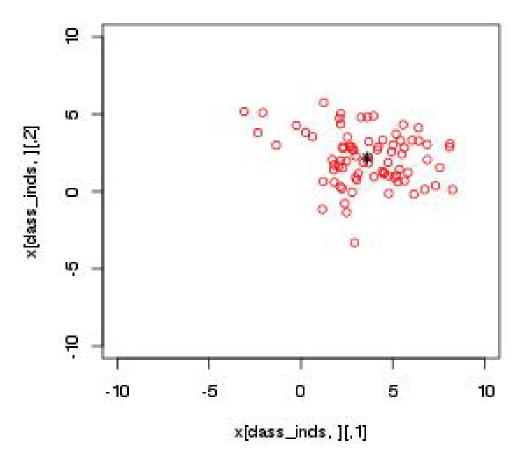
The EM Algorithm

- EM algorithm:
 - expectation-maximization algorithm
- Generalization of k-means to probabilistic setting
- Similar iterative procedure
 - 1. Calculate cluster probability for each instance (expectation step)
 - 2. Estimate distribution parameters based on the cluster probabilities (maximization step)
- Cluster probabilities are stored as instance weights





Kmeans – unequal cluster variance

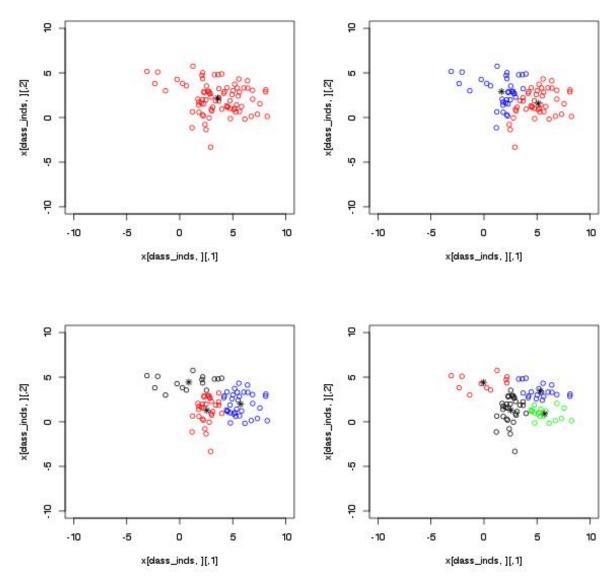


Can you guess K?





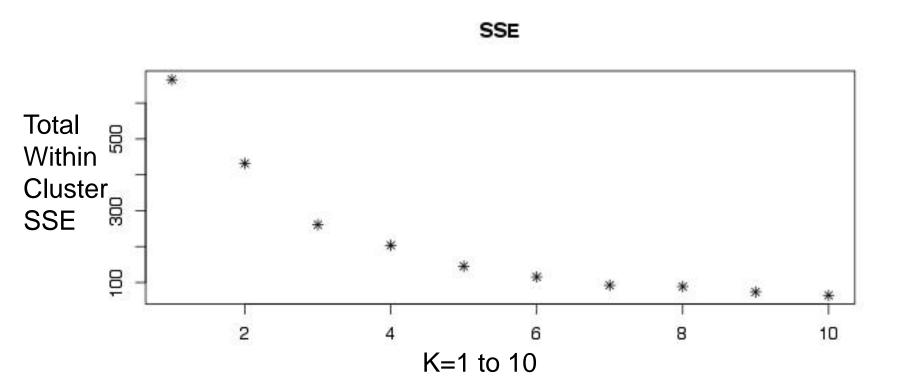
K-means – unequal cluster variance







Choosing K – unequal distributions



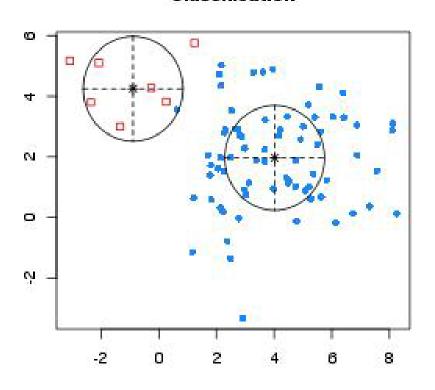
- Smooth decrease across K => less structure





EM clustering

Classification



- Selects K=2

 (either by Information Criterion=
 min of SSE+ K*logN,
 Or by cross-validation)
- Handles unequal variance





K-means computations

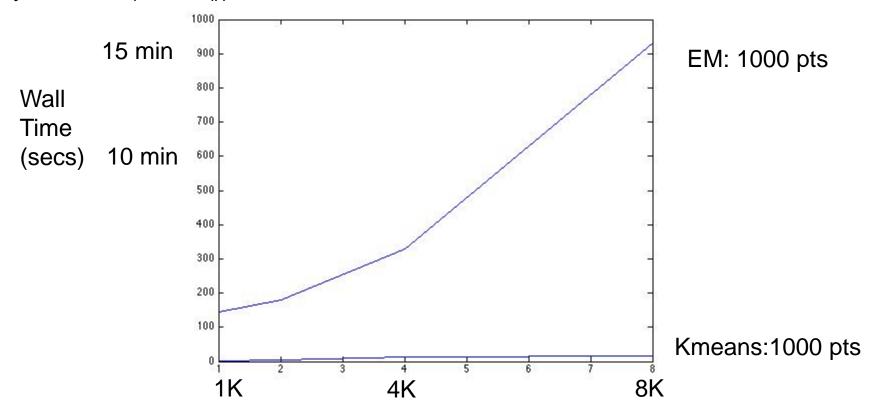
- Distance of each point to each cluster center
 - For N points, D dimensions: each loop requires N*D*K operations
- Update Cluster centers
 - only track points that change, get change in cluster center
- But for EM errors to each cluster center update a probability function





K-means vs EM performance

1 Gordon compute node, normal random matrices R: system.time(Mclust())



Number of Dimensions (i.e. columns in data matrix)





Kmeans big data example

45,000 NYTimes articles, 102,000 unique words

(UCI Machine Learning repository)

Full Data Matrix: 45Kx102K ~ 40Gb

article 1
article 2
article 3
...

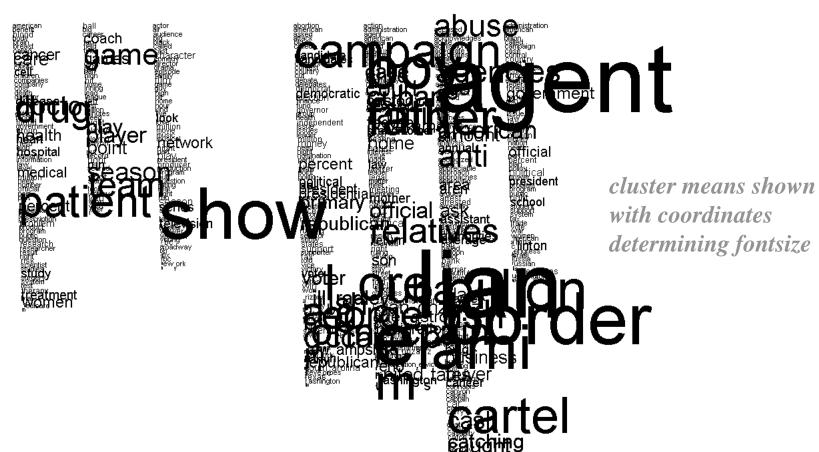
article 45K

Cell i,j is count of ith-word in jth-article





Kmeans results



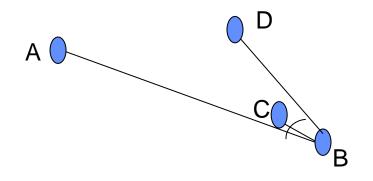
7 viable clusters found





Other distance measures

Cosine: each row is treated as vector in R^p, then take angles



C is closer to A because ABC°<ABD°

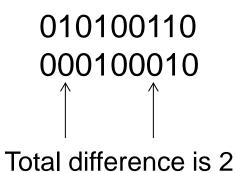
Jaccard (over sets A,B):

1- (|A∩B| / |AUB|)



Other distance measures

 Hamming distance: count 1 if values different e.g. appropriate for binary strings







Summary

- Labeled clusters can be interpreted by using supervised learning - train a tree or learn rules
- Can be used to fill in missing attribute values
- All methods have a basic assumption of independence between the attributes
 - Some methods allow the user to specify in advanced that two of more attributes are dependent and should be modeled with a joint probability





Clustering algorithms in scikit-learn

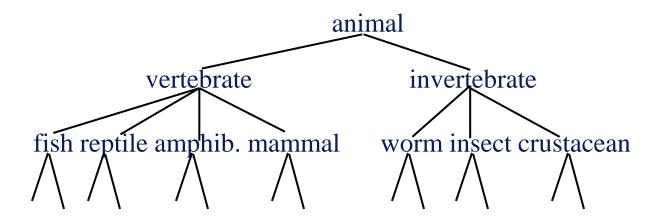
Method name	Parameters	Scalability	Usecase	Geometry (metric used)
<u>K-Means</u>	number of clusters	Very large n_samples, medium n_clusters with <u>MiniBatch code</u>	General-purpose, even cluster size, flat geometry, not too many clusters	Distances between points
Affinity propagation	damping, sample preference	Not scalable with n_samples	Many clusters, uneven cluster size, non-flat geometry	Graph distance (e.g. nearest-neighbor graph)
Mean-shift	bandwidth	Not scalable with n_samples	Many clusters, uneven cluster size, non-flat geometry	Distances between points
<u>Spectral</u> <u>clustering</u>	number of clusters	Medium n_samples, small n_clusters	Few clusters, even cluster size, non-flat geometry	Graph distance (e.g. nearest-neighbor graph)
Ward hierarchica clustering	number of clusters	Large n_samples and n_clusters	Many clusters, possibly connectivity constraints	Distances between points
Agglomerative clustering	number of clusters, linkage type, distance	Large n_samples and n_clusters	Many clusters, possibly connectivity constraints, non Euclidean distances	Any pairwise distance
<u>DBSCAN</u>	neighborhood size	Very large n_samples, medium n_clusters	Non-flat geometry, uneven cluster sizes	Distances between nearest points
<u>Gaussian</u> <u>mixtures</u>	many	Not scalable	Flat geometry, good for density estimation	Mahalanobis distances to centers
<u>Birch</u>	branching factor, threshold, optional global clusterer.	Large n_clusters and n_samples	Large dataset, outlier removal, data reduction.	Euclidean distance between points





Hierarchical Clustering

 Build a tree-based hierarchical taxonomy (dendrogram) from a set of unlabeled examples



 Recursive application of a standard clustering algorithm can produce a hierarchical clustering





Incremental & Hierarchical Clustering

- Start with 1 cluster (all instances) and do splits
 OR
 Start with N clusters (1 per instance) and do merges
- Can be greedy & expensive in its search
 some algorithms might merge & split
 algorithms need to store and recalculate distances
- Need distance between groups in contrast to K-means





Incremental & Hierarchical Clustering

Result is a hierarchy of clusters

displayed as a 'dendrogram' tree

Useful for tree-like interpretations

- syntax (e.g. word co-occurences)
- concepts (e.g. classification of animals)
- topics (e.g. sorting Enron emails)
- spatial data (e.g. city distances)
- genetic expression (e.g. possible biological networks)
- exploratory analysis





Incremental Clustering

- Works incrementally instance by instance forming a a hierarchy of clusters
- COBWEB nominal; CLASSIT numeric attributes
- Instances are added one at the time
 - Tree is updated appropriately at each step
 - Finding the right leaf for an instance
 - Restructuring the tree
- How and where to update based on category utility value





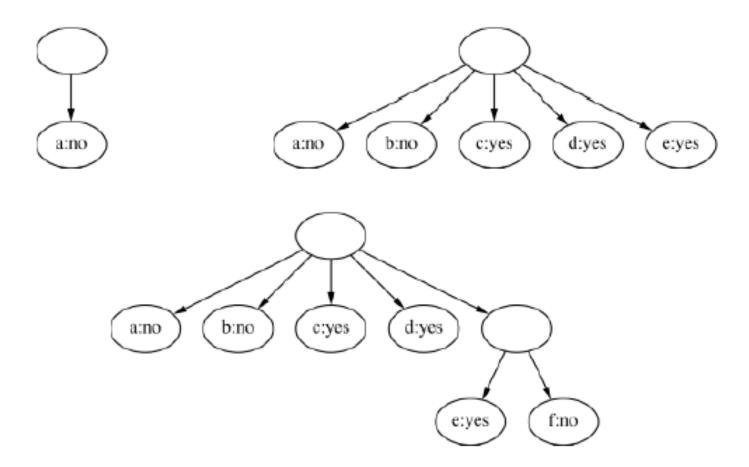
Clustering: Weather Data

Weather Data Set							
ID Code	Outlook	Temperature	Humidity	Windy			
Α	Sunny	Hot	High	False			
В	Sunny	Hot	High	True			
С	Overcast	Hot	High	False			
D	Rain	Mild	High	False			
E	Rain	Cool	Normal	False			
F	Rain	Cool	Normal	True			
F	Overcast	Cool	Normal	True			
Н	Sunny	Mild	High	False			
1	Sunny	Cool	Normal	False			
J	Rain	Mild	Normal	False			
K	Sunny	Mild	Normal	True			
L	Overcast	Mild	High	True			
M	Overcast	Hot	Normal	False			
N	Rain	Mild	High	True			





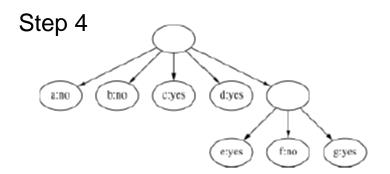
Clustering

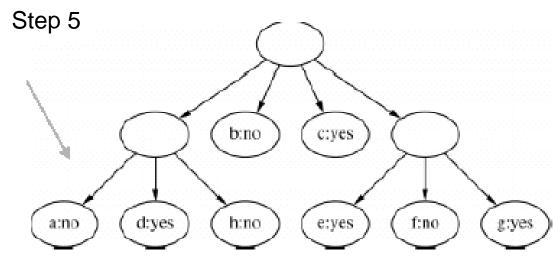






Clustering









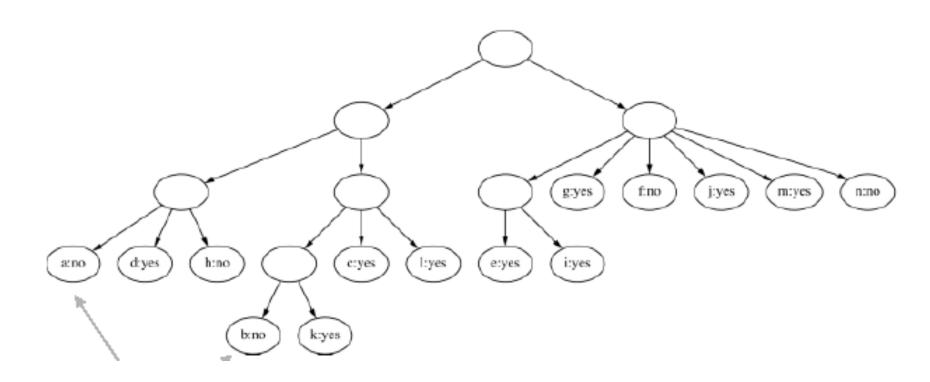
Merging

- Consider all pairs of nodes for merging and evaluate category utility of each
 - Computationally expensive
- When scanning nodes for a suitable host both the best matching node and the runner-up are noted
- The best will form the host for new instance unless merging host and runner-up produces better CU





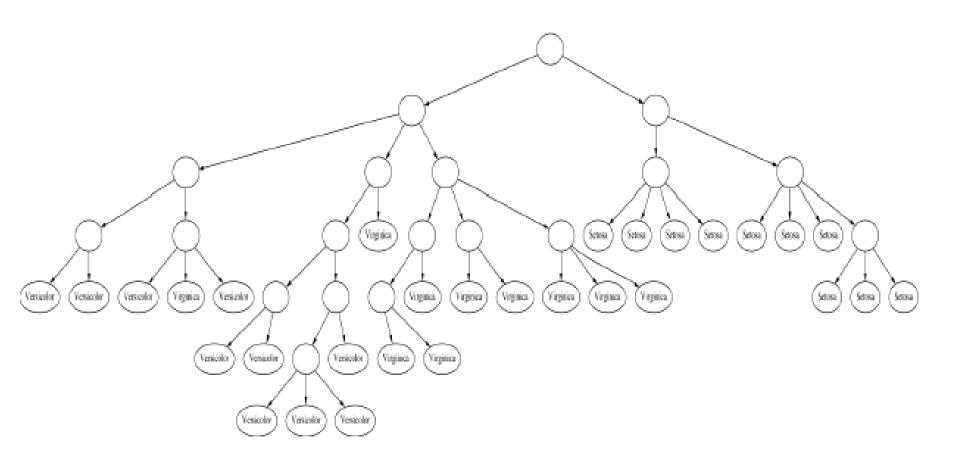
Final Hierarchy







Iris Data







Category utility

 Category utility is a kind of quadratic loss function defined on conditional probabilities:

$$CU(C_{1}, C_{2}, ..., C_{k}) = \frac{\sum_{l} \Pr[C_{l}] \sum_{i} \sum_{j} (\Pr[a_{i} = v_{ij} \mid C_{l}]^{2} - \Pr[a_{i} = v_{ij}]^{2})}{k}$$

- C₁, ..C_k are k clusters
- a_i is the *i*th attribute
- Takes on values v_{i1}, v_{i2}, ...





Category Utility Extended to Numeric Attributes

Assuming normal distribution:

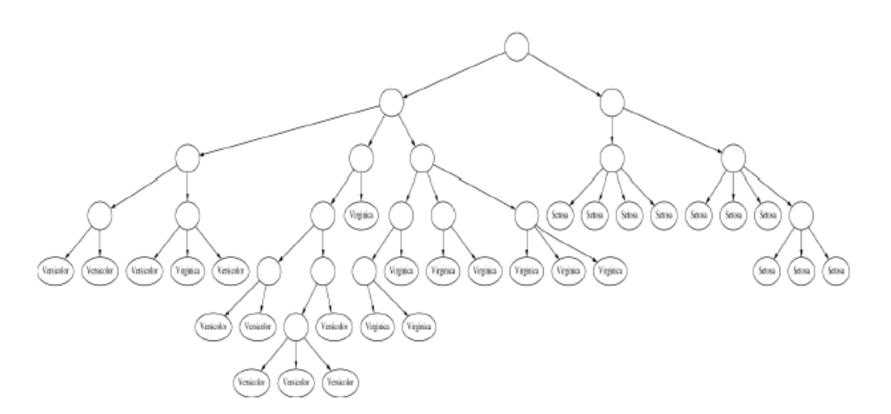
$$CU = \frac{\sum_{l} \Pr[C_{l}] \frac{1}{2\sqrt{\pi}} \sum_{i} \left(\frac{1}{\sigma_{il}} - \frac{1}{\sigma_{i}} \right)}{k}$$

- When Standard deviation of attribute a_i is zero it produced infinite value of the category utility formula
- Acuity parameter: pre-specified minimum variance on each attribute
 - only one instance in a node produces 0 variance





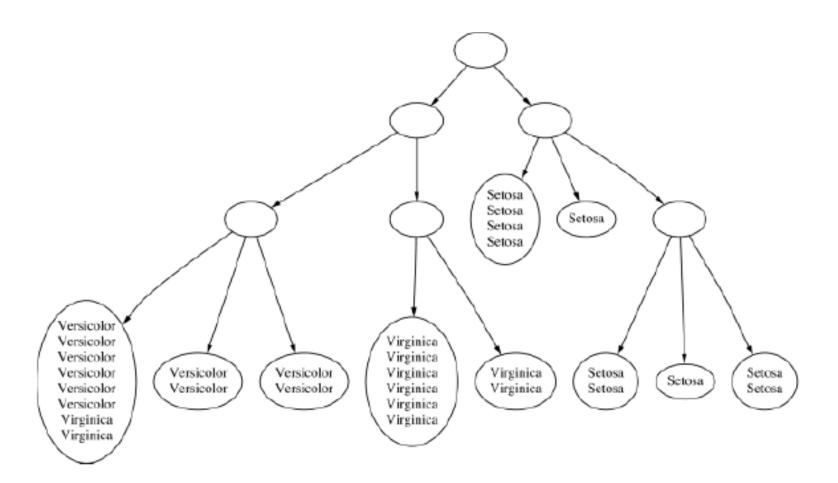
Iris Data Final Hierarchy







Clustering with Cutoff







Incremental & Hierarchical Clustering

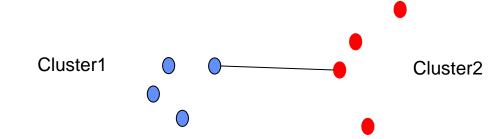
- Clusters are merged/split according to distance or utility measure
 - Euclidean distance (squared differences)
 - conditional probabilities (for nominal features)
- Options to choose which clusters to 'Link'
 - single linkage, mean, average (w.r.t. points in clusters)
 (may lead to different trees, depending on spreads)
 - Ward method (smallest increase within cluster variance)
 - change in probability of features for given clusters



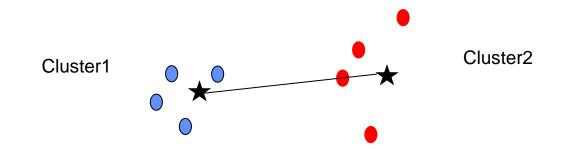


Linkage options

• e.g. single linkage (closest to any cluster instance)



• e.g. mean (closest to mean of all cluster instances)

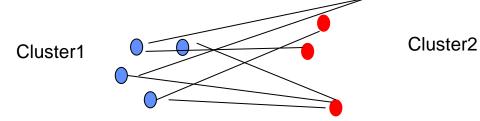




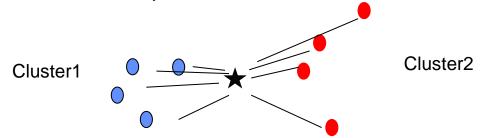


Linkage options (cont')

e.g. average (mean of pairwise distances)



e.g. Ward's method (find new cluster with min. variance)







Hierarchical Clustering Demo

3888 Interactions among 685 proteins

From Hu et.al. TAP dataset http://www.compsysbio.org/bacteriome/dataset/)

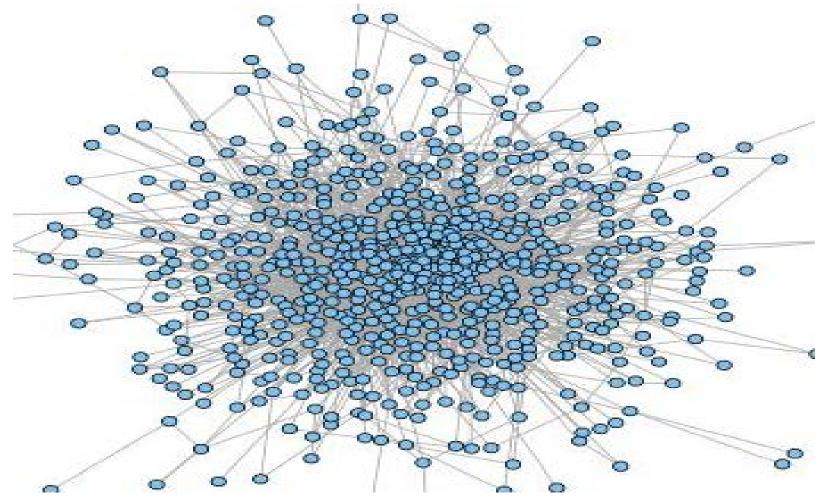
```
b0014
b0009
                0.92
b0009
        b2231
                0.87
b0014
        b0169
                1.0
b0014
       b0595
                0.76
       b2614
b0014
                1.0
b0014
       b3339
                0.95
b0014
        b3636
                0.9
b0015
        b0014
                0.99
```

.





Interactions as connections – structure is hard to see

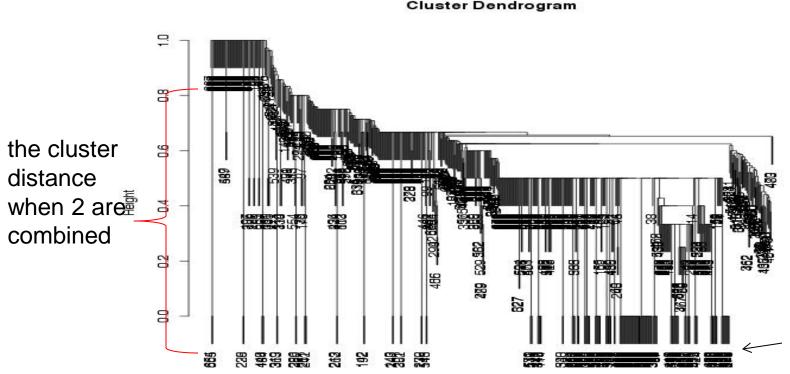






Hierarchical Clustering Demo

hclust with "single" distance: chaining



Items that cluster first

d2use hdust (*, "single")

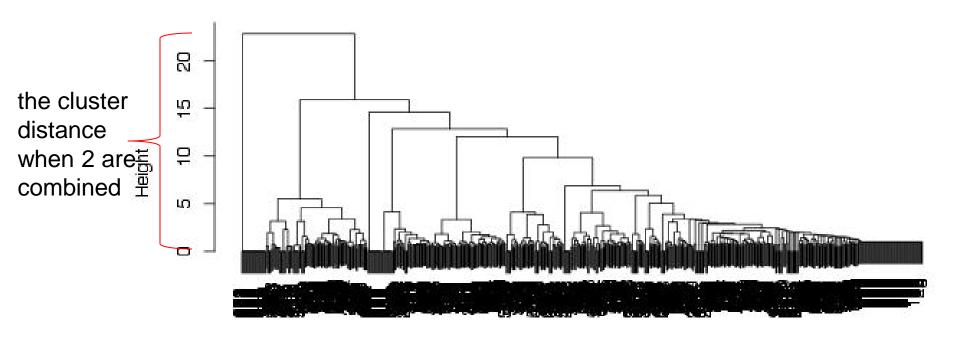




Hierarchical Clustering Demo

hclust with "Ward" distance: spherical clusters

Cluster Dendrogram



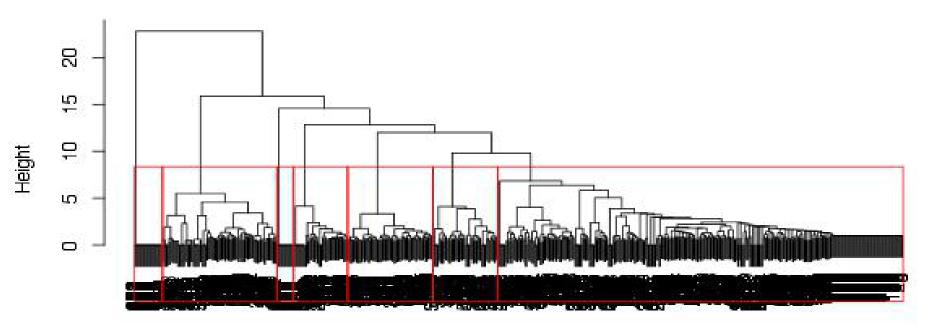




Hierarchical Clustering Demo

Where height change looks big, cut off tree

Cluster Dendrogram







Summary

- Having no label doesn't stop you from finding structure in data
- Labeled clusters can be interpreted by using supervised learning - train a tree or learn rules
- Can be used to fill in missing attribute values
- All methods have a basic assumption of independence between the attributes
 - Some methods allow the user to specify in advanced that two of more attributes are dependent and should be modeled with a joint probability
- Unsupervised methods are somewhat related





Exercise: Clustering Athlete's Data in Weka

Is there a relationship between athlete's physical attributes and their sport?

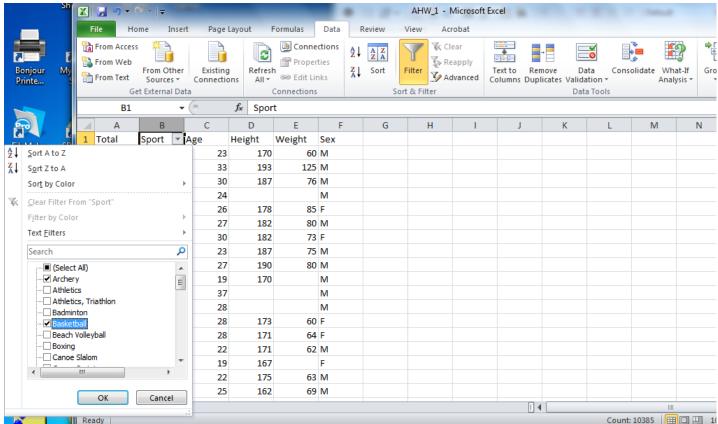
Let's filter data to try a few, good, candidate sport categories.





Weka not nice for picking out instances with multi-criteria, so I used excel: (Excel, data -> advanced -> click on column and then drop down selection menu. Include only a few sports)

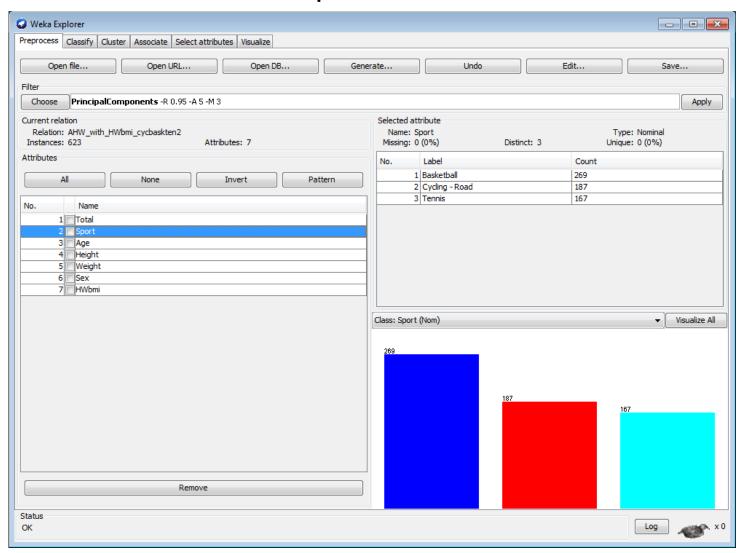
Download AHW_withHWbmi_cycbaskten2.csv from pace.sdsc.edu, open in weka







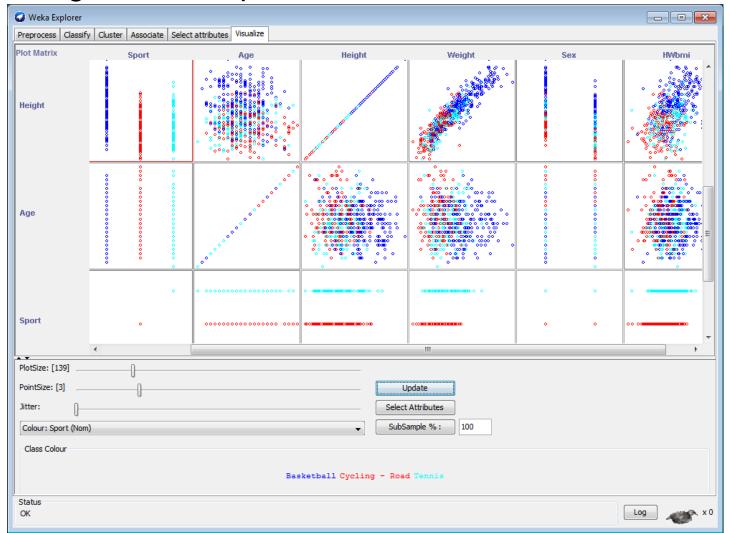
Notice the number of sports and their nominal values







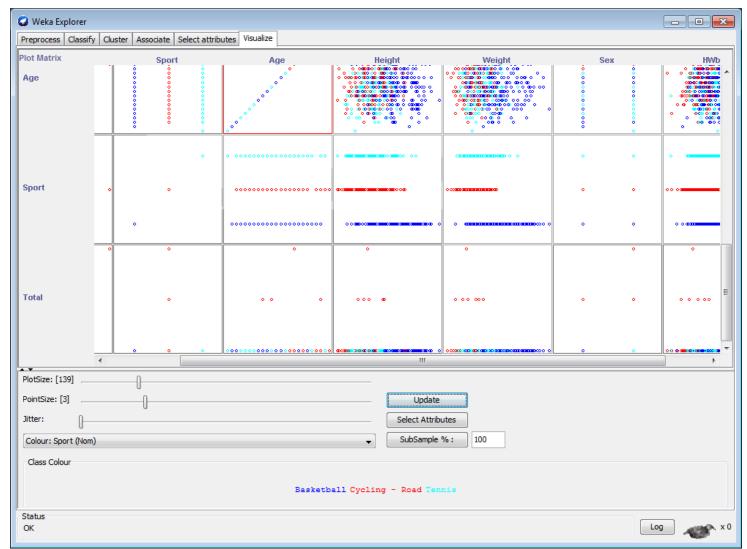
 Visualize correlation with sport as class – any problems, any promising relationships?







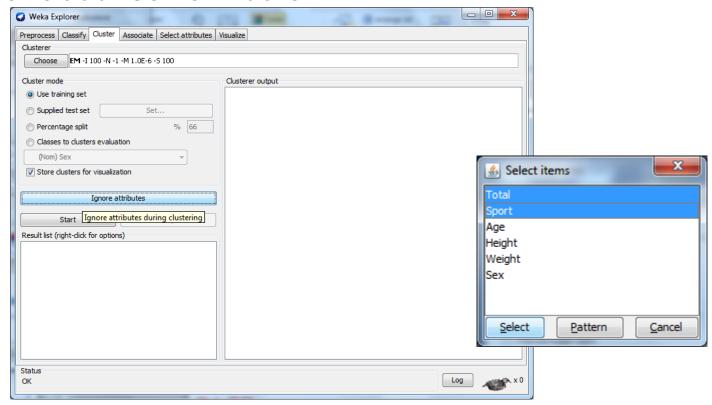
Are there one or more variables we should ignore?







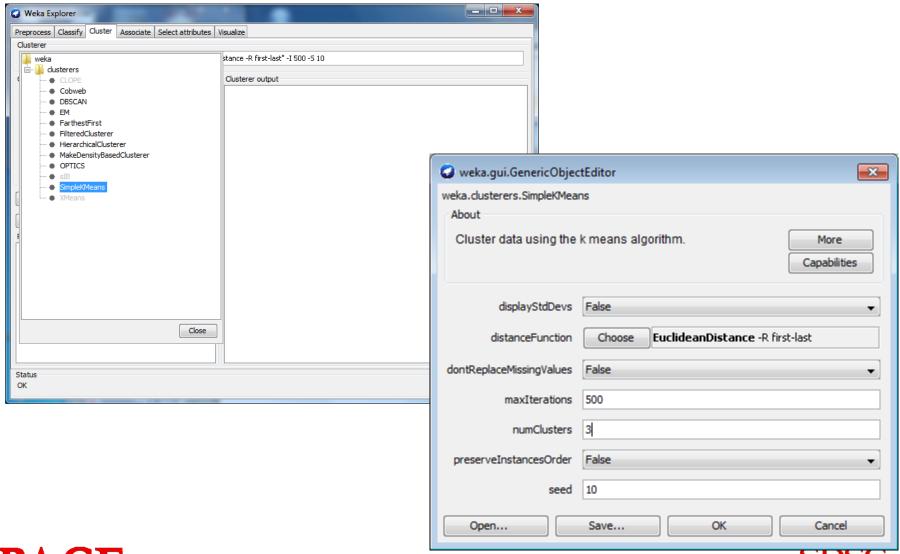
Select Ignore attributes -> ctrl-space to ignore sport (why?) and total medals won (why or why not?) What about sex attribute?



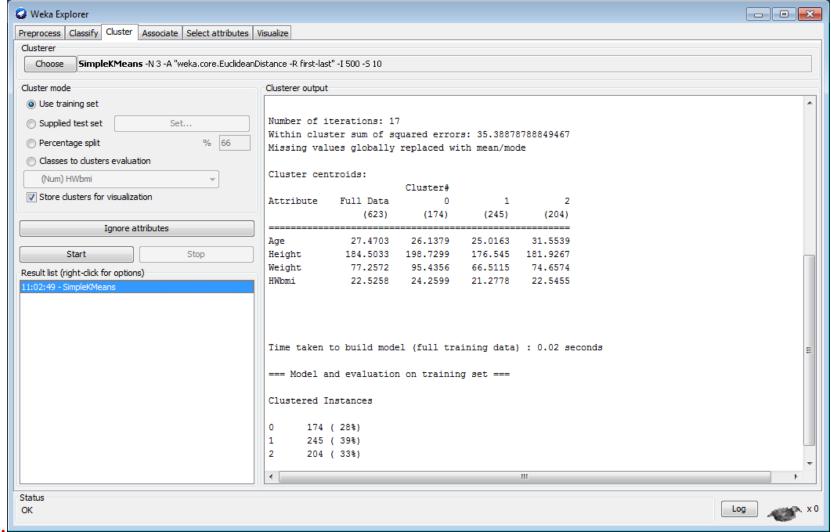




select cluster tab; choose -> simple Kmeans; choose 3 classes, accept other defaults

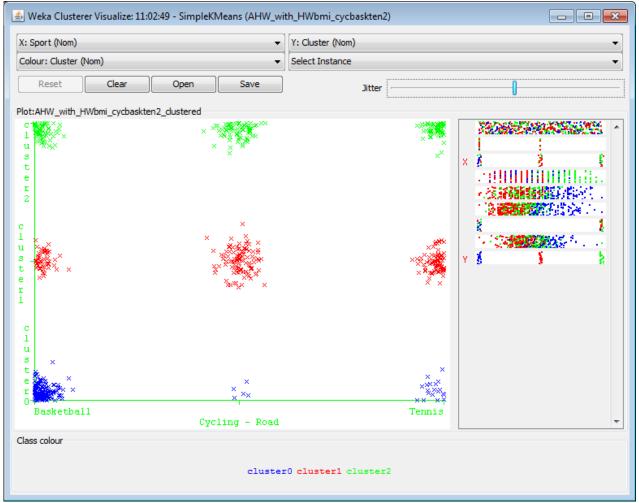


Results end up in output panel. Take note of sum squared error. Any other message to note?





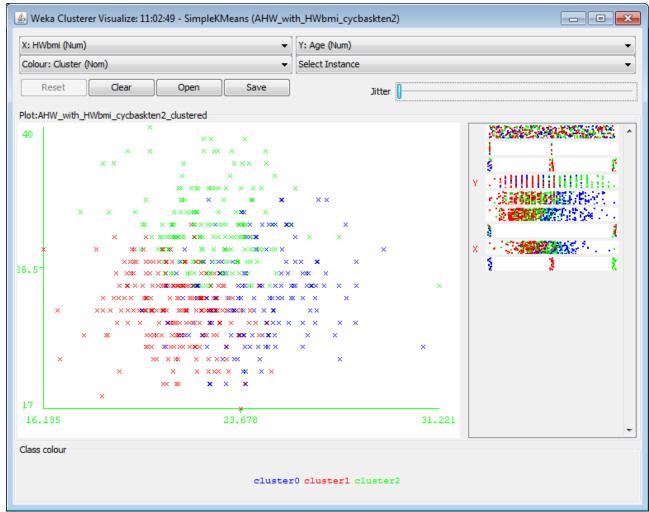
Rt click on model result, visualize cluster assignment, add jitter Compare sport and cluster number – how do they correspond? Are the clusters useful to distinguish (or predict) an athlete's sport?





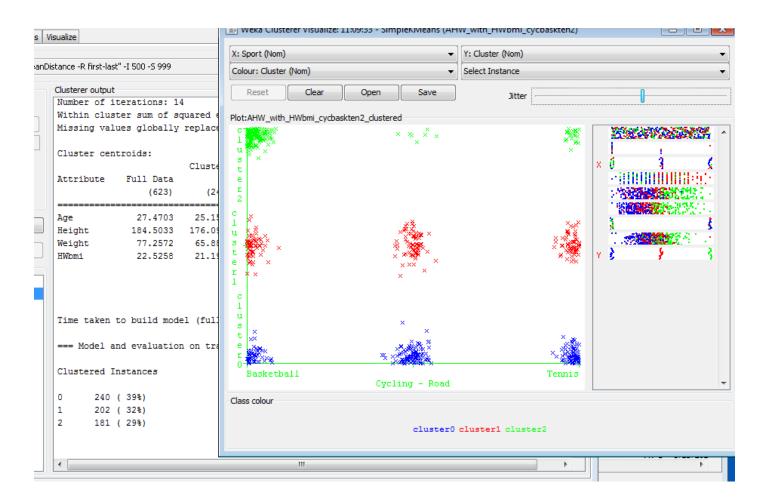


Compare clusters in the 2 dimension subspace of BMI and Age - (or any other subspace)





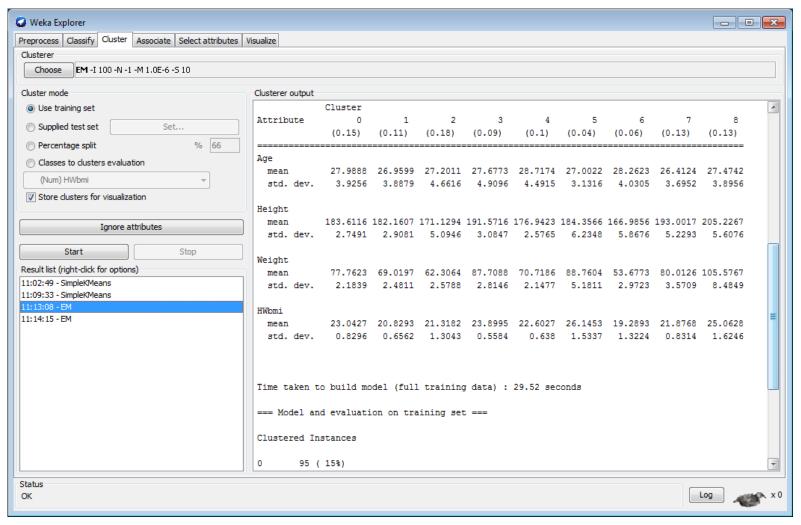
Try rerunning with different random seed, you get different clustering, but similar SSE







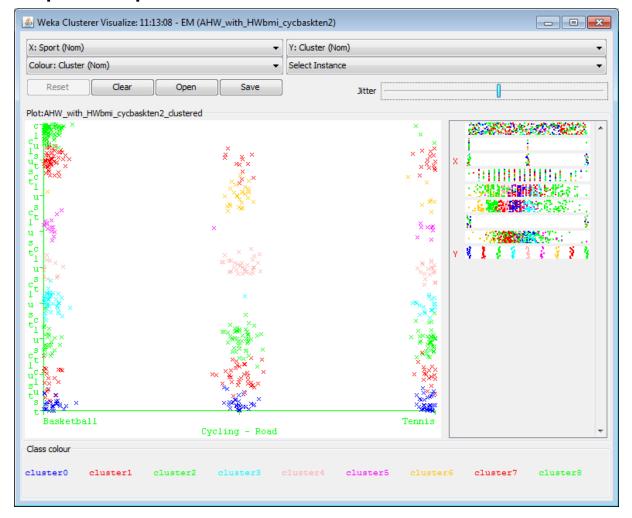
Try EM algorithm, accept defaults and start







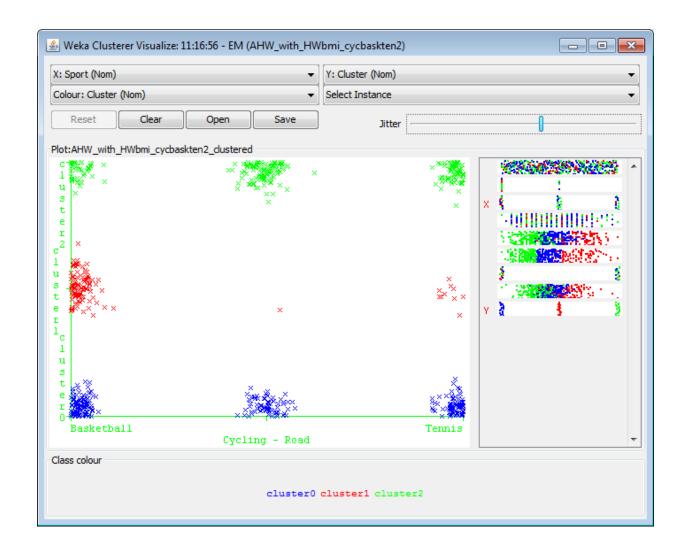
Rt click on model result, visualize cluster assignment, Compare sport and cluster number







Rerun with 5 clusters, compare sport and cluster number







Exercise:

For simple Kmeans Get a full sweep of K – ie change N to 1,3,4,5, what K would you choose?



