Data Mining
Lecture 3: Discovering Groups

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Discovering Groups - Introduction

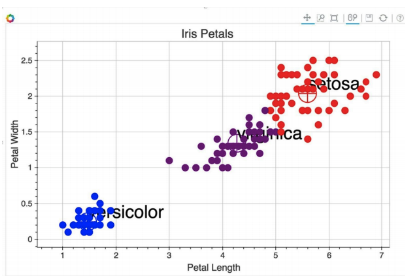
Understanding large datasets is hard, especially if it has high dimensional features
To help understand a dataset:

- Find similar data items
- Find similar features

Discovering Groups - Clustering

Grouping data, just using the feature vectors

- Unsupervised
- Similar feature vectors grouped together
- Can be
  - Soft (allow overlapping groups)
  - Hard (each item assigned to one group)



Discovering Groups - K Means

Algorithm 1: K Means clustering

Data: X, K
initialise K centroids;
while *positions of centroids change* **do**
  for *each data point* **do**
    assign to nearest centroid;
  end
  for *each centroid* **do**
    move to average of assigned data points
  end
end
return centroids, assignments;

A special case of Expectation Maximisation
K Means ipynb demo
K Means Java Demo

Discovering Groups - Hierarchical Clustering

Hierarchical Clustering:

Creates a binary tree that recursively groups pairs of similar items or clusters

Can be:

- Agglomerative (bottom up)
- Divisive (top down)

Discovering Groups - Hierarchical Clustering

Algorithm 2: Hierarchical Agglomerative Clustering

Data: N data points with feature vectors X_i $i = 1 \dots N$

$numClusters = N$;

while $numClusters > 1$ **do**

  cluster1, cluster2 = FindClosestClusters();

  merge(cluster1, cluster2);

end

The distance between the clusters is evaluated using a linkage criterion.
If each merge is recorded, a binary tree structure linking the clusters can be formed.
This gives a **dendrogram**

Discovering Groups - Hierarchical Clustering

Linkage criterion: A measure of dissimilarity between clusters
Centroid Based:

- Dissimilarity is equal to distance between centroids
- Needs numeric feature vectors

Distance-Based:

- Dissimilarity is a function of distance between items in clusters
- Only needs precomputed measure of similarity between items

We could compute a distance matrix between points

Discovering Groups - Hierarchical Clustering

Centroid based linkage:

- WPGMC: Weighted Pair Group Method with Centroids
  When two clusters are combined into a new cluster, the average of the two centroids is the new centroid
- UPGMC: Unweighted Pair Group Method with Centroids
  When two clusters are combined into a new cluster, the new centroid is recalculated based on the positions of the items

Discovering Groups - Hierarchical Clustering

Distance based linkage:

- **Minimum**, or **single-linkage clustering** Distance between two closest members

$$\min d(a,b) : a \in A, b \in B$$

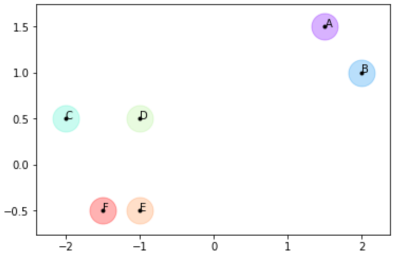
  Produces long, thin clusters
- **Maximum**, or **complete-linkage clustering** Distance between two most distant members

$$\max d(a,b) : a \in A, b \in B$$

  Finds compact clusters, approximately equal diameter
- **Mean** or **Average Linkage Clustering** (**UPGMA**: Unweighted Pairwise Group Method with Arithmetic Mean):

$$\frac{1}{|A||B|}\sum_{a\in A}\sum_{b\in B} d(a,b)$$

Discovering Groups - Hierarchical Clustering



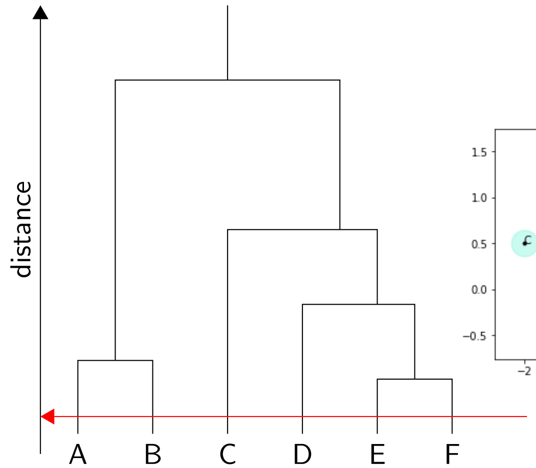
With sample data:

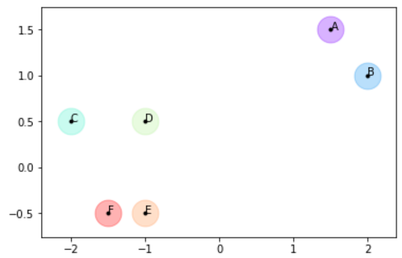
$$X = \begin{bmatrix} 1.5 & 1.5 \\ 2.0 & 1.0 \\ 2.0 & 0.5 \\ -1.0 & 0.5 \\ -1.5 & -0.5 \\ -1 & 0.5 \end{bmatrix}$$

Distance matrix:

	A	B	C	D	E	F
A	0	0.7	2.7	1.8	...	
B	0.7	0	...			
C	2.7		0	...		
D	1.8			0	...	
E	⋮				0	
F	⋮					0

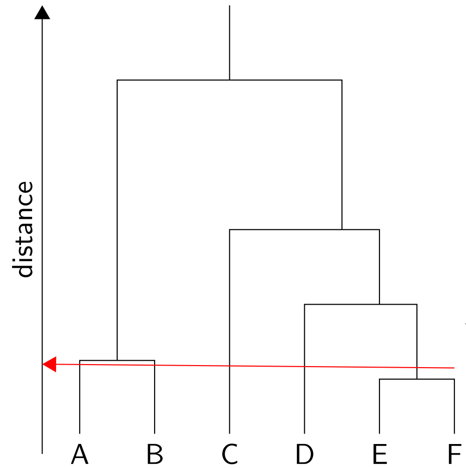
Discovering Groups - Centroid Clustering

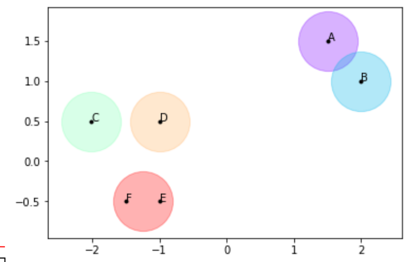




Using minimum or single-linkage clustering

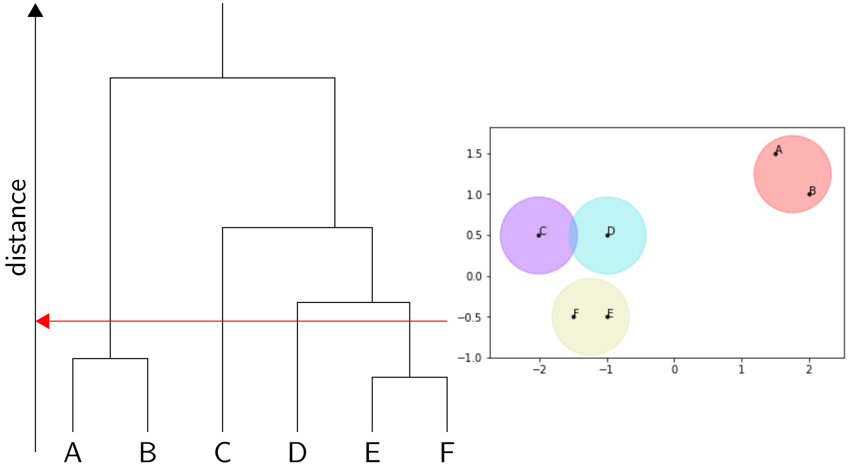
Discovering Groups - Centroid Clustering





Using minimum or single-linkage clustering

Discovering Groups - Centroid Clustering



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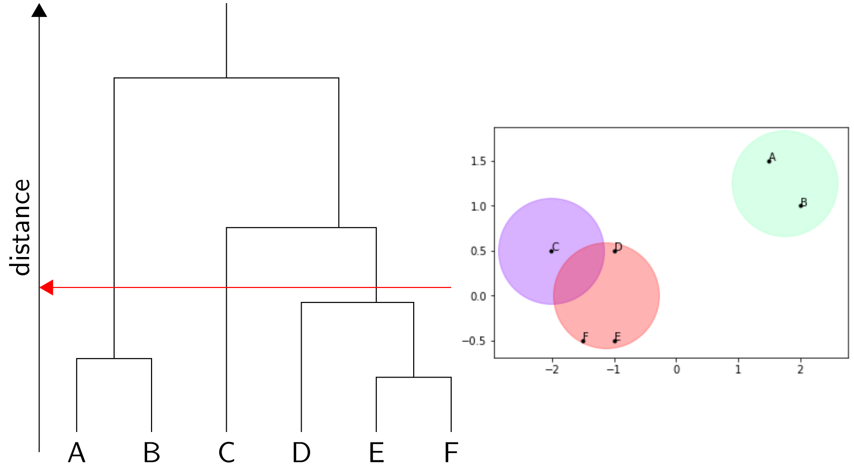
Discovering Groups - Centroid Clustering



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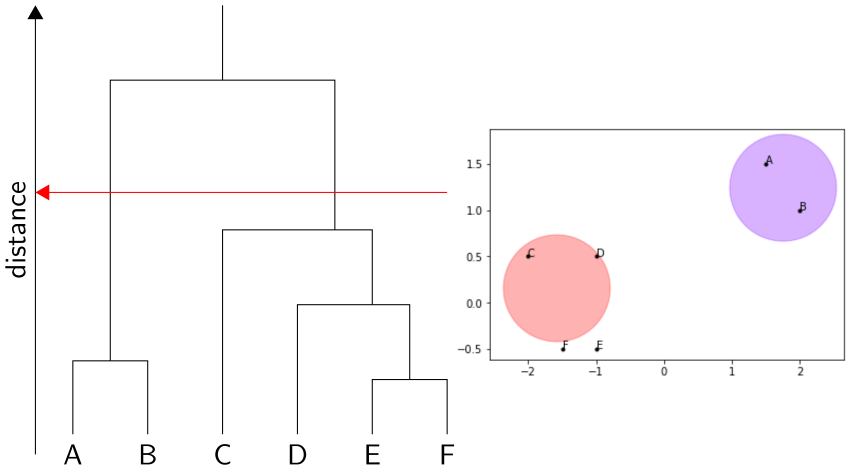

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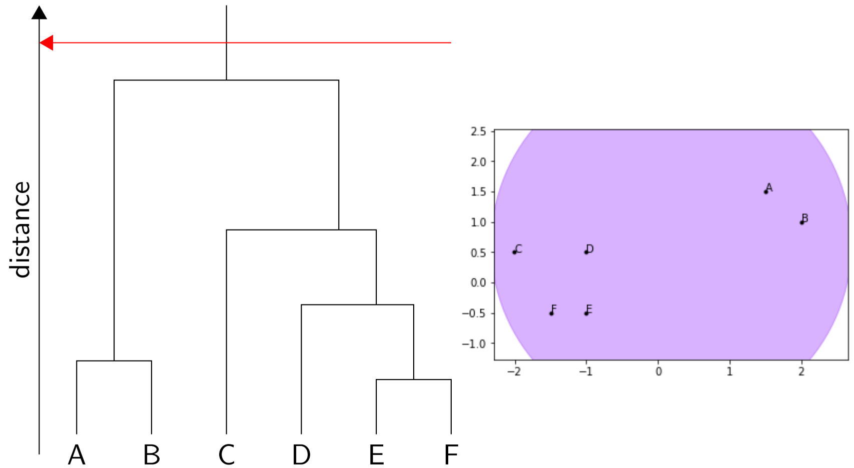

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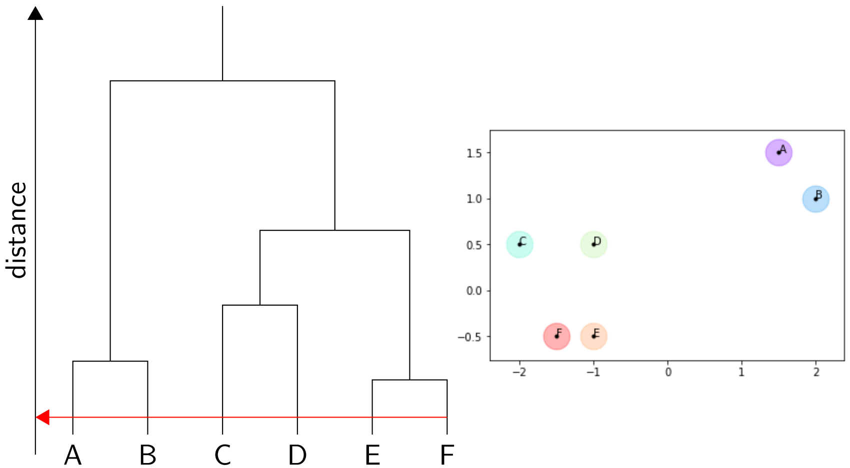
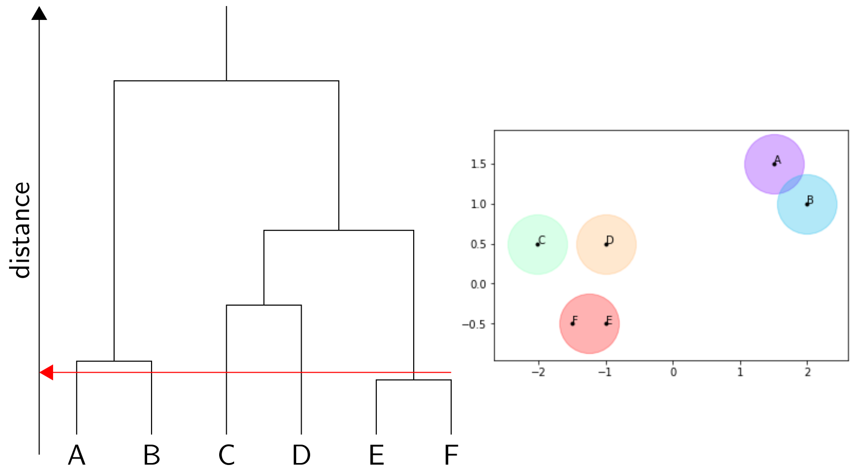
Discovering Groups - Centroid Clustering



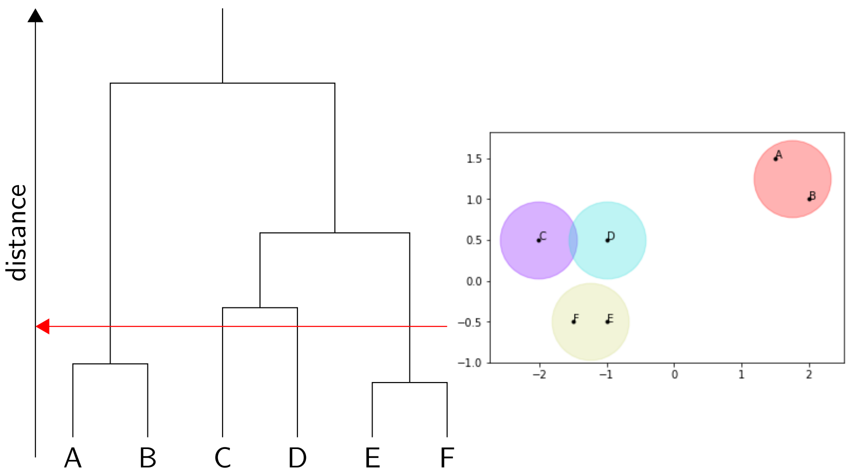
Using maximum or complete-linkage clustering

Discovering Groups - Centroid Clustering



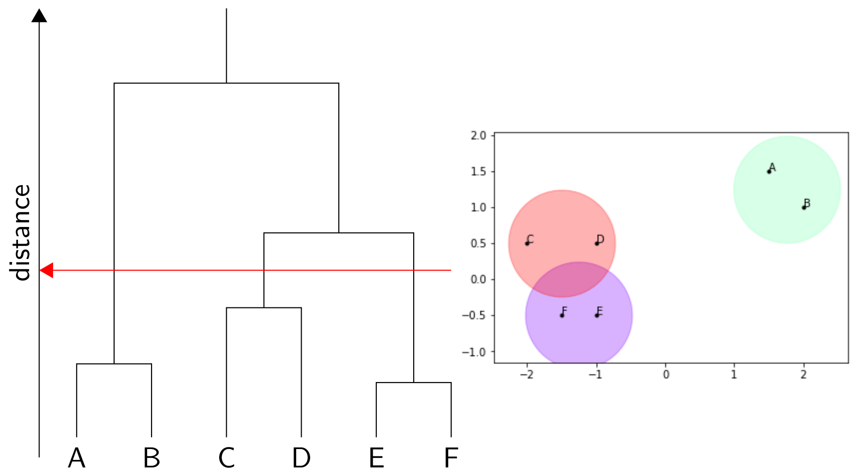
Using maximum or complete-linkage clustering

Discovering Groups - Centroid Clustering



Using maximum or complete-linkage clustering

Discovering Groups - Centroid Clustering



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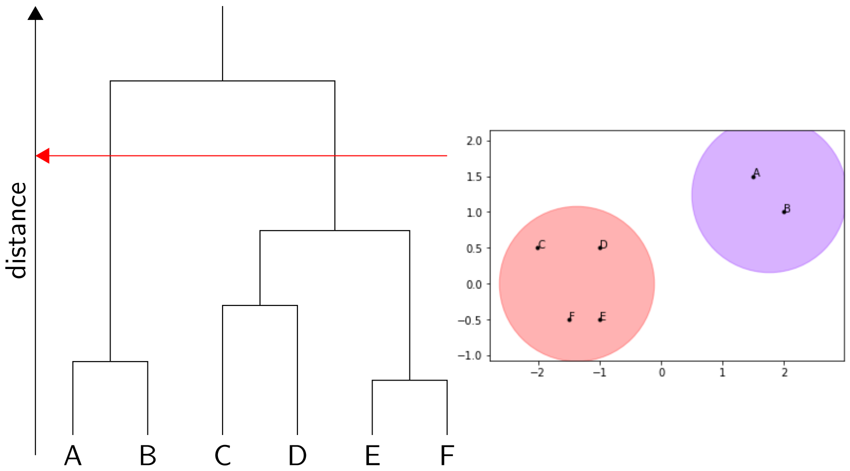
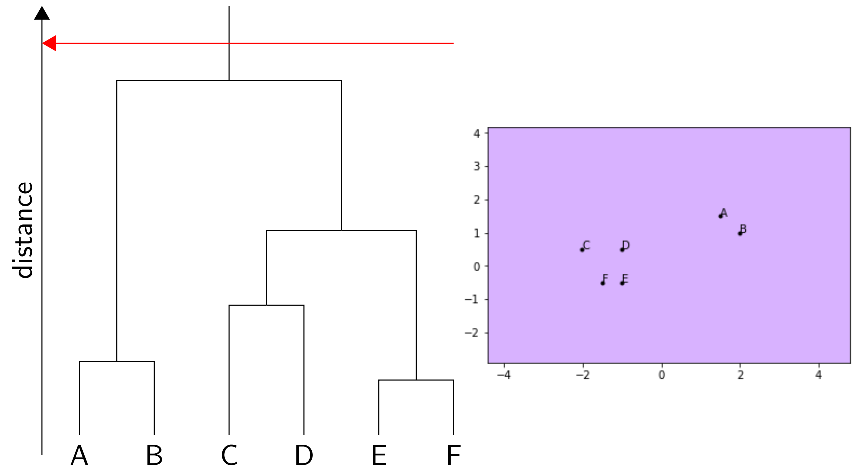
Discovering Groups - Centroid Clustering



Using maximum or complete-linkage clustering

Discovering Groups - Centroid Clustering



Using maximum or complete-linkage clustering

Discovering Groups - Hierarchical Agglomerative Clustering

Java HAC Demo
Minimum distance linkage tends to give long thin clusters
maximum distance linkage tends to give rounded clusters

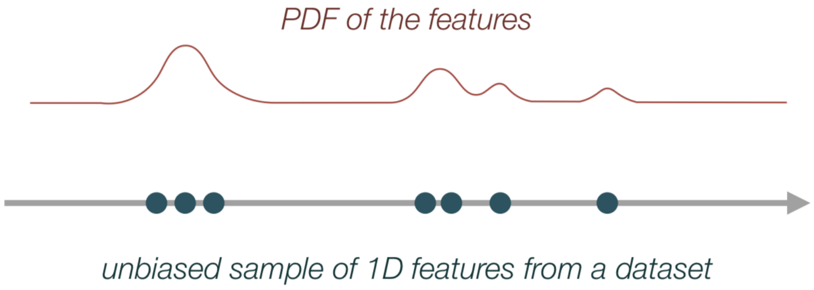
Discovering Groups - Mean Shift Clustering

Mean shift finds the *modes* of a probability density function.

This means if finds the points in feature space with the highest feature density, i.e. are the most likely given the dataset
Needs a kernel and a kernel bandwidth.

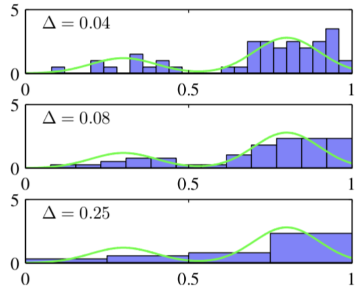
It is a hill climbing algorithm that

Discovering Groups - Mean Shift Clustering



Discovering Groups - Mean Shift Clustering

How can we estimate the PDF?
Could use a histogram, need to guess number of bins



Changing bin size affecting accuracy of probability density estimation[1]

Can be too crude

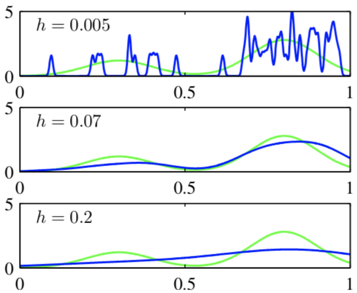
[1] C. Bishop, Pattern Recognition and Machine Learning

Discovering Groups - Mean Shift Clustering

Kernel Density Estimation (aka Parzen Window)
Gives a smooth continuous estimate

$$f(x) = \frac{1}{nh^d}\sum_{i=1}^{n} K(\frac{x - x_i}{h})$$

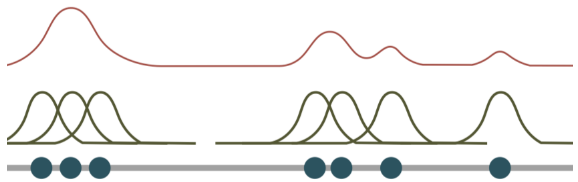
Where nh is the number of items, d is the dimensionality of the feature space, K is the kernel function, x is an arbitrary position in feature space, h is the kernel bandwidth



Changing bandwidth affecting accuracy of probability density estimation

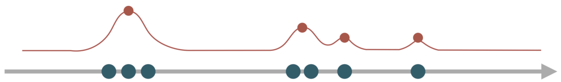
Discovering Groups - Mean Shift Clustering

Usually use a Gaussian kernel with $\sigma = 1$
If kernel is radially symmetric, then only need profile of kernel, $k(x)$ that satisfies $K(x) = C_{k,d}k(||x||^2)$



Discovering Groups - Mean Shift Clustering

Find the modes of the probability density function (PDF), i.e. where the gradient is zero. $\Delta f(x) = 0$



Discovering Groups - Mean Shift Clustering

$$f(x) = \frac{1}{nh^d} \sum_{i=1}^{n} K(\frac{x - x_i}{h})$$

$$K(x) = c_{k,d} k(||x||^2)$$

Where $c_{k,d}$ is a normalisation constant

$$f(x) = \frac{c_{k,d}}{nh^d} \sum_{i=1}^{n} k(||\frac{x - x_i}{h}||^2)$$

Assuming a radially symmetric kernel:

$$\Delta f(x) = \frac{2c_{k,d}}{nh^{d+2}} \sum_{i=1}^{n} (x - x_i) g(||\frac{x - x_i}{h}||^2) \quad g(x) = -k'(x)$$

$$\Delta f(x) = \frac{2c_{k,d}}{nh^{d+2}} \sum_{i=1}^{n} g(||\frac{x - x_i}{h}||^2) \frac{\sum_{i=1}^{n} x_i g(||\frac{x-x_i}{h}||^2)}{\sum_{i=1}^{n} g(||\frac{x-x_i}{h}||^2)} - x$$

Discovering Groups - Mean Shift Clustering

$$\Delta f(x) = \frac{2c_{k,d}}{nh^{d+2}} \sum_{i=1}^{n} g(||\frac{x-x_i}{h}||^2) \frac{\sum_{i=1}^{n} x_i g(||\frac{x-x_i}{h}||^2)}{\sum_{i=1}^{n} g(||\frac{x-x_i}{h}||^2)} - x$$

The first part is a probability density estimate with kernel $G(x) = x_{g,d} g(||x||^2)$

Discovering Groups - Mean Shift Clustering

$$\Delta f(x) = \frac{2c_{k,d}}{nh^{d+2}} \sum_{i=1}^{n} g(||\frac{x - x_i}{h}||^2) \frac{\sum_{i=1}^{n} x_i g(||\frac{x-x_i}{h}||^2)}{\sum_{i=1}^{n} g(||\frac{x-x_i}{h}||^2)} - x$$

The first part is a probability density estimate with kernel $G(x) = x_{g,d} g(||x||^2)$

The second part is the mean shift, the vector that always points in the direction of maximum density

Discovering Groups - Mean Shift Clustering

Mean shift algorithm:

Algorithm 3: Mean Shift Procedure

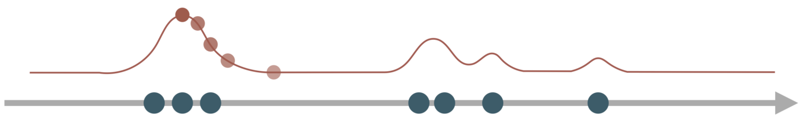
Data: N data points with feature vectors $X_i \; i = 1 \dots N$

while $x_t not = x_{t+1}$ **do**

  $m_h(x_t) = \text{computeMeanShiftVect}();$

  $x_{t+1} = x_t + m_h(x_t);$

end

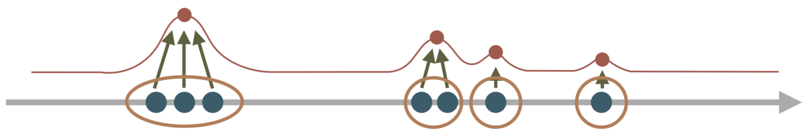


Discovering Groups - Mean Shift Clustering

For each feature vector:

- apply mean shift procedure until convergence
- store resultant mode

Set of feature vectors that converge to the same mode define the basin of attraction of that mode



Discovering Groups - Summary

Clustering is a key way to understand your data.

There are many different approaches

- K Means - Need to chose K
- Hierarchical Agglomerative Clustering -
- Mean Shift Clustering

They are a very good way to start exploring a dataset
Coursework 2 is Set!