Unsupervised Clustering

Digging into Data

April 14, 2014

COLLEGE OF INFORMATION STUDIES

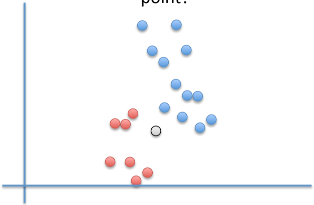
Slides adapted from Lauren Hannah

Lecture for Today

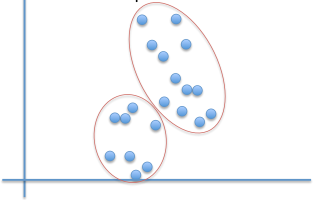
- What is clustering?
- K-Means
- R's implementation of K-means
- Write a K-means algorithm in R
- Animations in R

Clustering

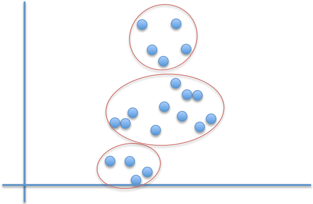
Classification: what is label of new point?



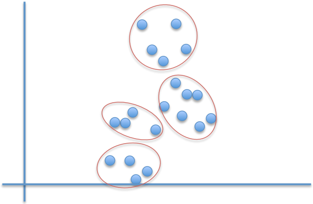
Clustering: how should we group these points?



Clustering: or is this the right grouping?



Clustering: what about this?

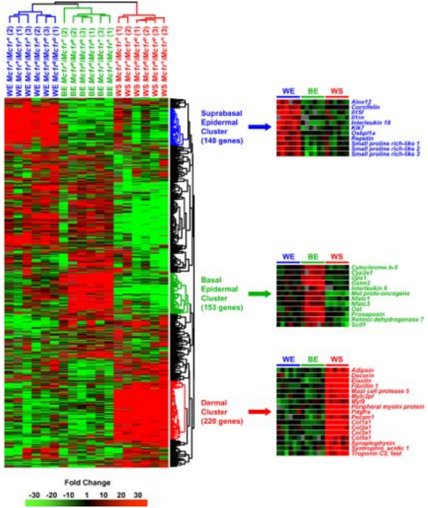


Clustering

Uses:

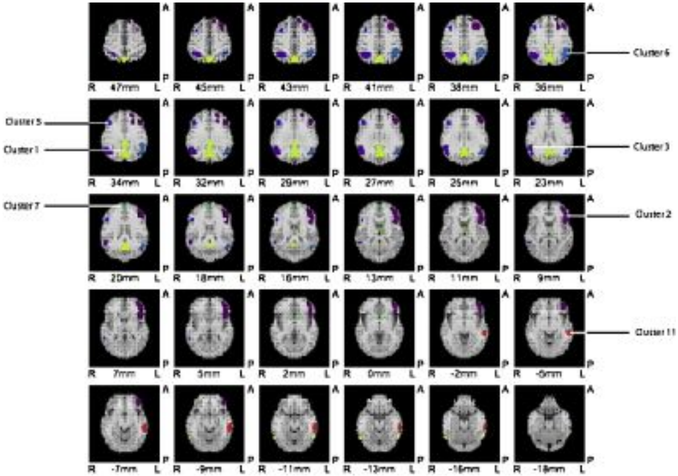
- genomics
- medical imaging
- social network analysis
- recommender systems
- market segmentation
- voter analysis

Microarray Gene Expression Data



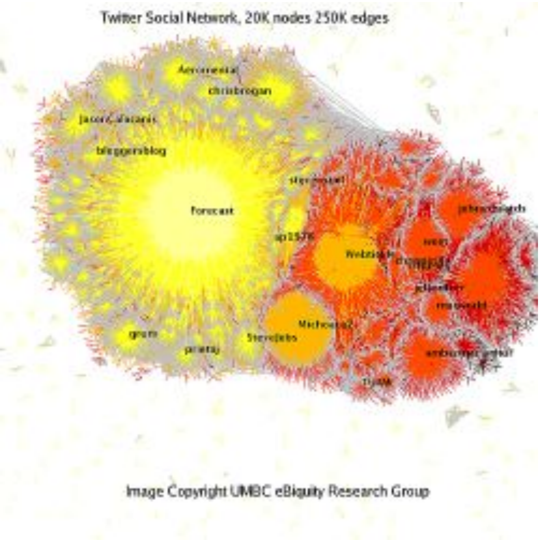
From: “Skin layer-specific transcriptional profiles in normal and recessive yellow (Mc1re/Mc1re) mice” by April and Barsh in *Pigment Cell Research* (2006)

Medical Imaging (MRIs and PET scans)



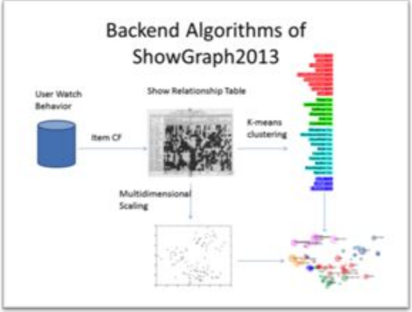
From: "Fluorodeoxyglucose positron emission tomography of mild cognitive impairment with clinical follow-up at 3 years" by Pardo et al. in *Alzheimer's and Dementia* (2010)

Social Networks



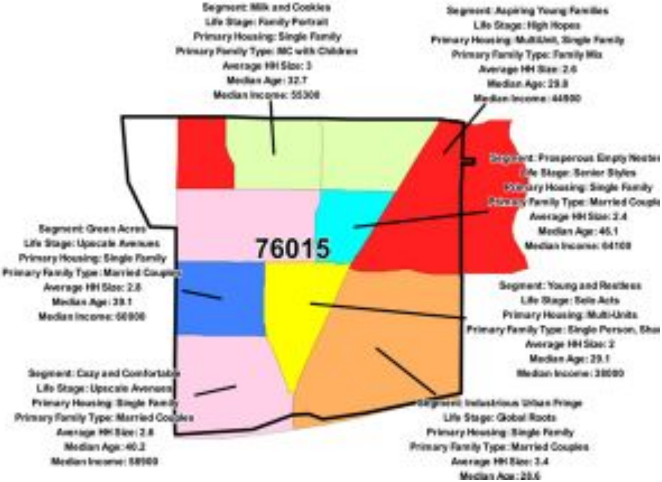
From: http://flowingdata.com/2008/03/12/17-ways-to-visualize-the-twitter-universe/

Recommender Systems



From: tech.hulu.com/blog/

Market Segmentation



From: mappinganalytics.com/map/segmentation-maps/segmentation-map.html

Voter Analysis

- soccer moms (female, middle aged, married, middle income, white, kids, suburban)
- Nascar dads (male, middle aged, married, middle income, white, kids, Southern, suburban or rural)
- security moms (...)
- low information voters

- Ivy League Elites

Clustering

Questions:

- how do we fit clusters?
- how many clusters should we use?
- how should we evaluate model fit?

K-Means

How do we fit the clusters?

- simplest method: K-means
- requires: real-valued data
- idea:
  - pick K initial cluster means
  - associate all points closest to mean k with cluster k
  - use points in cluster k to update mean for that cluster
  - re-associate points closest to new mean for k with cluster k
  - use new points in cluster k to update mean for that cluster
  - ...
  - stop when no change between updates

K-Means

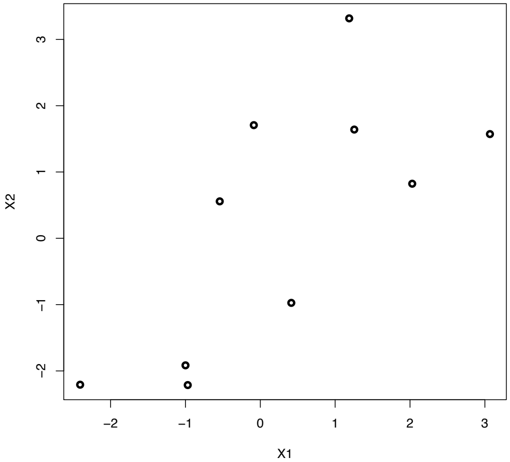
Animation at:

`http://animation.yihui.name/mvstat:k-means_cluster_algorithm`

K-Means: Example

Data:

x_1	x_2
0.4	-1.0
-1.0	-2.2
-2.4	-2.2
-1.0	-1.9
-0.5	0.6
-0.1	1.7
1.2	3.3
3.1	1.6
1.3	1.6
2.0	0.8

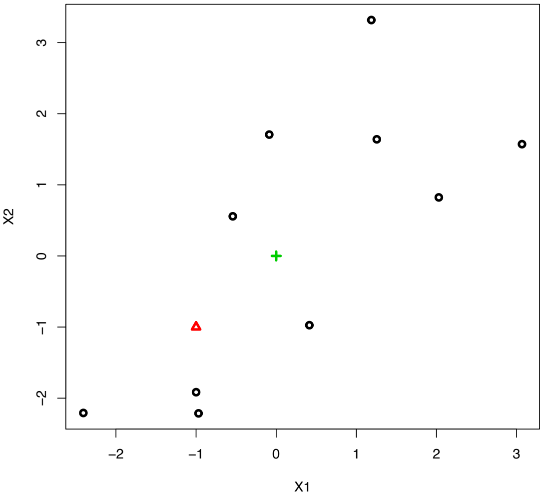



```
> # Data
> x
```

K-Means: Example

Pick K centers (randomly):

$$(-1,-1) \text{ and } (0,0)$$



K-Means: Example

Calculate distance between points and those centers:

x_1	x_2	$(-1,-1)$	$(0,0)$
0.4	-1.0	1.4	1.1
-1.0	-2.2	1.2	2.4
-2.4	-2.2	1.9	3.3
-1.0	-1.9	0.9	2.2
-0.5	0.6	1.6	0.8
-0.1	1.7	2.9	1.7
1.2	3.3	4.8	3.5
3.1	1.6	4.8	3.4
1.3	1.6	3.5	2.1
2.0	0.8	3.5	2.2

```
> centers <- rbind(c(-1,-1),c(0,0))
> dist1 <- apply(x,1,function(x) sqrt(sum((x-centers[1,])^2)))
> dist2 <- apply(x,1,function(x) sqrt(sum((x-centers[2,])^2)))
```

K-Means: Example

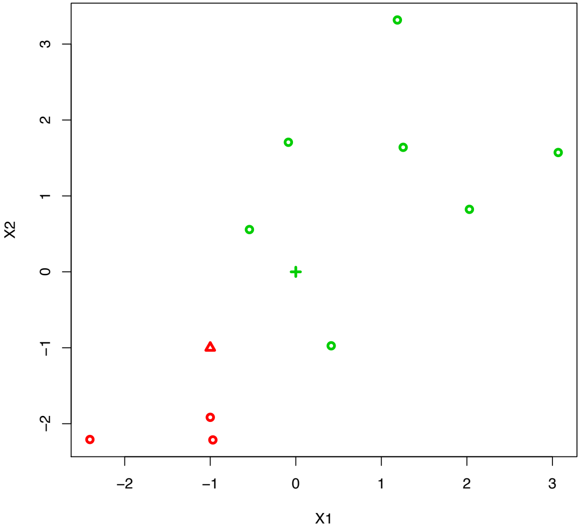
Choose mean with smaller distance:

x_1	x_2	$(-1,-1)$	$(0,0)$
0.4	-1.0	1.4	**1.1**
-1.0	-2.2	**1.2**	2.4
-2.4	-2.2	**1.9**	3.3
-1.0	-1.9	**0.9**	2.2
-0.5	0.6	1.6	**0.8**
-0.1	1.7	2.9	**1.7**
1.2	3.3	4.8	**3.5**
3.1	1.6	4.8	**3.4**
1.3	1.6	3.5	**2.1**
2.0	0.8	3.5	**2.2**

```
> dists <- cbind(dist1,dist2)
> cluster.ind <- apply(dists,1,which.min)
```

K-Means: Example

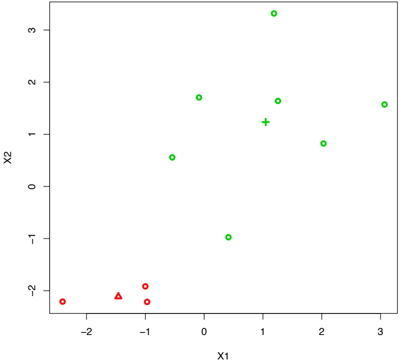
New clusters:



K-Means: Example

Refit means for each cluster:

- cluster 1: $(-1.0, -2.2)$, $(-2.4, -2.2)$, $(-1.0, -1.9)$
- new mean: $(-1.5, -2.1)$
- cluster 2: $(0.4, -1.0)$, $(-0.5, 0.6)$, $(-0.1, 1.7)$, $(1.2, 3.3)$, $(3.1, 1.6)$, $(1.3, 1.6)$, $(2.0, 0.8)$
- new mean: $(1.0, 1.2)$



K-Means: Example

Recalculate distances for each cluster:

x_1	x_2	$(-1.5, -2.1)$	$(1.0, 1.2)$
0.4	-1.0	2.2	2.3
-1.0	-2.2	0.5	4.0
-2.4	-2.2	1.0	4.9
-1.0	-1.9	0.5	3.8
-0.5	0.6	2.8	1.7
-0.1	1.7	4.1	1.2
1.2	3.3	6.0	2.1
3.1	1.6	5.8	2.0
1.3	1.6	4.6	0.5
2.0	0.8	4.6	1.1

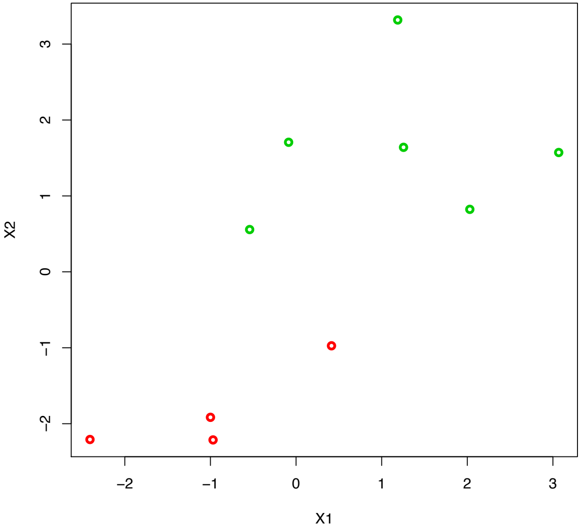
K-Means: Example

Choose mean with smaller distance:

x_1	x_2	$(-1.5, -2.1)$	$(1.0, 1.2)$
0.4	-1.0	**2.2**	2.3
-1.0	-2.2	**0.5**	4.0
-2.4	-2.2	**1.0**	4.9
-1.0	-1.9	**0.5**	3.8
-0.5	0.6	2.8	**1.7**
-0.1	1.7	4.1	**1.2**
1.2	3.3	6.0	**2.1**
3.1	1.6	5.8	**2.0**
1.3	1.6	4.6	**0.5**
2.0	0.8	4.6	**1.1**

K-Means: Example

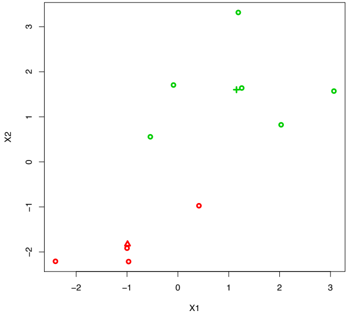
New clusters:



K-Means: Example

Refit means for each cluster:

- cluster 1: $(0.4, -1.0)$, $(-1.0, -2.2)$, $(-2.4, -2.2)$, $(-1.0, -1.9)$
- new mean: $(-1.0, -1.8)$
- cluster 2: $(-0.5, 0.6)$, $(-0.1, 1.7)$, $(1.2, 3.3)$, $(3.1, 1.6)$, $(1.3, 1.6)$, $(2.0, 0.8)$
- new mean: $(1.2, 1.6)$



K-Means: Example

Recalculate distances for each cluster:

x_1	x_2	$(-1.0, -1.8)$	$(1.2, 1.6)$
0.4	-1.0	1.6	2.7
-1.0	-2.2	0.4	4.4
-2.4	-2.2	1.5	5.2
-1.0	-1.9	0.1	4.1
-0.5	0.6	2.4	2.0
-0.1	1.7	3.6	1.2
1.2	3.3	5.6	1.7
3.1	1.6	5.3	1.9
1.3	1.6	4.1	0.1
2.0	0.8	4.0	1.2

K-Means: Example

Select smallest distance and compare these clusters with previous:

Table : New Clusters

x_1	x_2	$(-1.0, -1.8)$	$(1.2, 1.6)$
0.4	-1.0	**1.6**	2.7
-1.0	-2.2	**0.4**	4.4
-2.4	-2.2	**1.5**	5.2
-1.0	-1.9	**0.1**	4.1
-0.5	0.6	2.4	**2.0**
-0.1	1.7	3.6	**1.2**
1.2	3.3	5.6	**1.7**
3.1	1.6	5.3	**1.9**
1.3	1.6	4.1	**0.1**
2.0	0.8	4.0	**1.2**

Table : Old Clusters

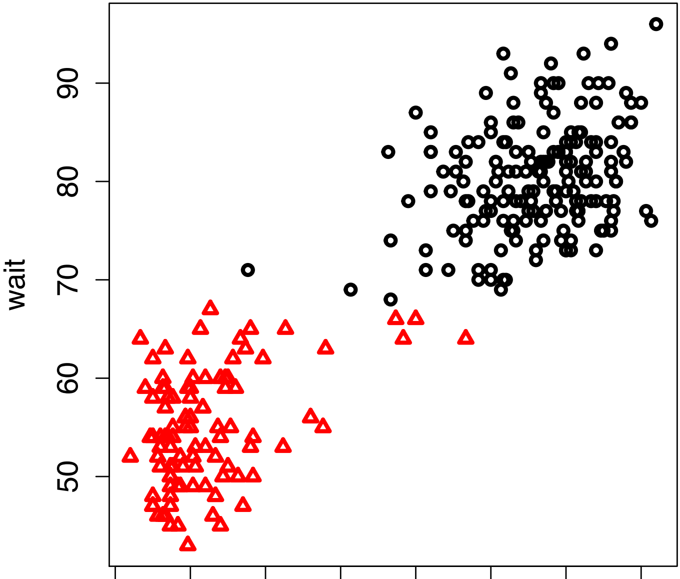
$(-1.5, -2.1)$	$(1.0, 1.2)$
2.2	2.3
0.5	4.0
1.0	4.9
0.5	3.8
2.8	**1.7**
4.1	**1.2**
6.0	**2.1**
5.8	**2.0**
4.6	**0.5**
4.6	**1.1**

K-Means in R

R has a function for K-means in the stats package; this is probably already loaded

- let's use this for the Old Faithful data

```
> library(datasets)
> faith.2 <- kmeans(faithful,2)
> names(faith.2)
> plot(faithful[,1],faithful[,2],col=faith.2$cluste
 +   pch=faith.2$cluster,lwd=3)
```


wait
90
80
70
60
50

K-Means in R

K-means can be used for *image segmentation*

- partition image into multiple segments
- find boundaries of objects
- make art

Limitations of k-means

k-means is fast and simple, but ...

- What if your data are discrete?
- What if each data point has more than one cluster? (digits vs. documents)
- What if you don't know the number of clusters?