Clustering

Machine Learning: Jordan Boyd-Graber

University of Maryland

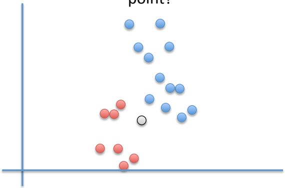
K-MEANS AND GMM

Lecture for Today

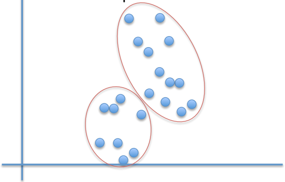
- What is clustering?
- K-Means
- Gaussian Mixture Models

Clustering

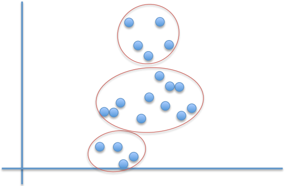
Classification: what is label of new point?



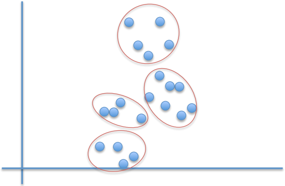
Clustering: how should we group these points?



Clustering: or is this the right grouping?



Clustering: what about this?

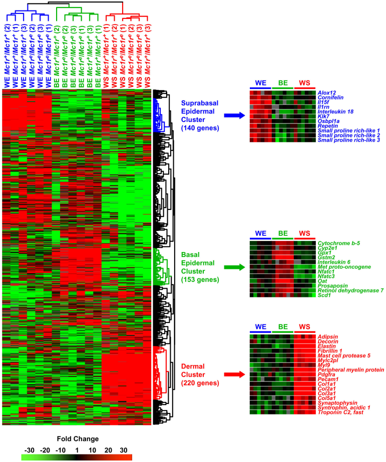


Clustering

Uses:

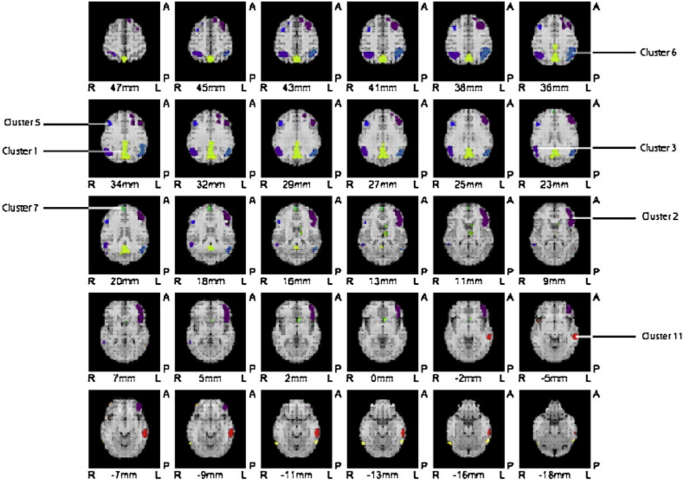
- genomics
- medical imaging
- social network analysis
- recommender systems
- market segmentation
- voter analysis

Microarray Gene Expression Data



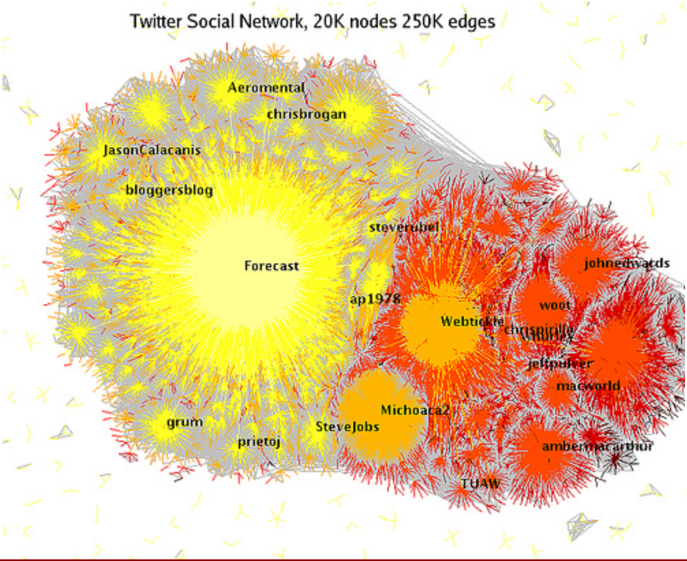
From: "Skin layer-specific transcriptional profiles in normal and recessive yellow (Mc1re/Mc1re) mice" by April and Barsh in *Pigment Cell Research* (2006)

Medical Imaging (MRIs and PET scans)

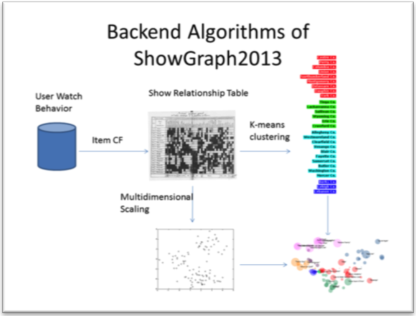


From: “Fluorodeoxyglucose positron emission tomography of mild cognitive impairment with clinical follow-up at 3 years” by Pardo et al. in *Alzheimer’s and Dementia* (2010)

Social Networks



Recommender Systems



Backend Algorithms of ShowGraph2013

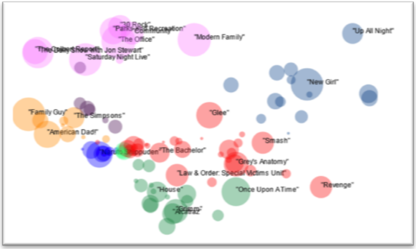
User Watch Behavior

Item CF

Show Relationship Table

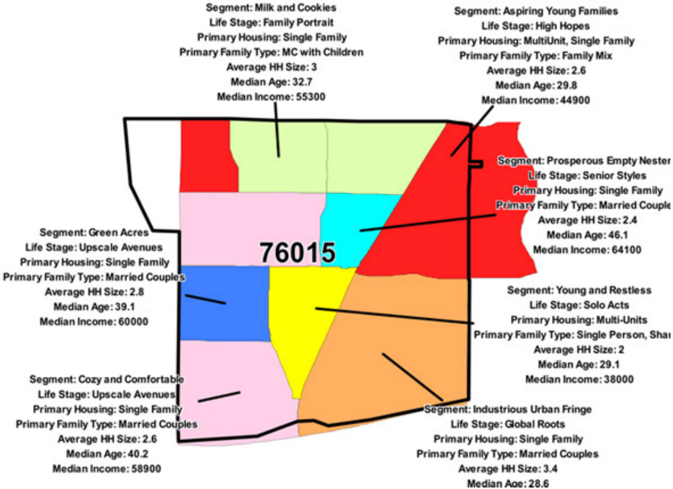
K-means clustering

Multidimensional Scaling



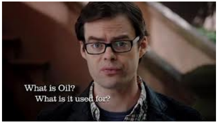
From: tech.hulu.com/blog/

Market Segmentation


Segment: Milk and Cookies
Life Stage: Family Portrait
Primary Housing: Single Family
Primary Family Type: MC with Children
Average HH Size: 3
Median Age: 32.7
Median Income: 55300
Segment: Aspiring Young Families
Life Stage: High Hopes
Primary Housing: MultiUnit, Single Family
Primary Family Type: Family Mix
Average HH Size: 2.6
Median Age: 29.8
Median Income: 44900
Segment: Prosperous Empty Nester
Life Stage: Senior Styles
Primary Housing: Single Family
Primary Family Type: Married Couple
Average HH Size: 2.4
Median Age: 46.1
Median Income: 64100
Segment: Green Acres
Life Stage: Upscale Avenues
Primary Housing: Single Family
Primary Family Type: Married Couples
Average HH Size: 2.8
Median Age: 39.1
Median Income: 60000
76015
Segment: Young and Restless
Life Stage: Solo Acts
Primary Housing: Multi-Units
Primary Family Type: Single Person, Sha
Average HH Size: 2
Median Age: 29.1
Median Income: 38000
Segment: Cozy and Comfortable
Life Stage: Upscale Avenues
Primary Housing: Single Family
Primary Family Type: Married Couples
Average HH Size: 2.6
Median Age: 40.2
Median Income: 58900
Segment: Industrious Urban Fringe
Life Stage: Global Roots
Primary Housing: Single Family
Primary Family Type: Married Couples
Average HH Size: 3.4
Median Age: 28.6

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

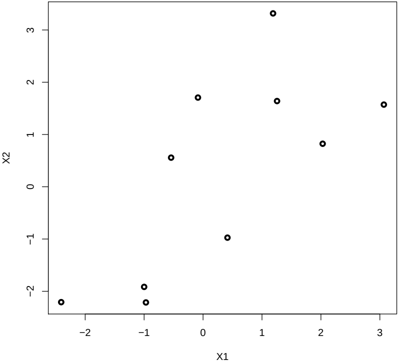
K-Means

Animation at:
`http://shabal.in/visuals/kmeans/1.html`

K-Means: Example

Data:

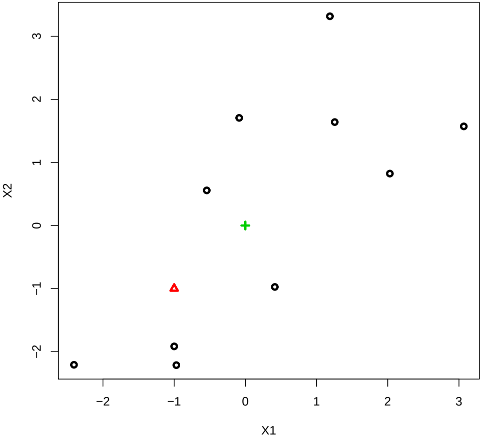
x_1	x_2
0.4	-1.0
-1.0	-2.2
-2.4	-2.2
-1.0	-1.9
-0.5	0.6
-0.1	1.7
1.2	3.3
3.1	1.6
1.3	1.6
2.0	0.8



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

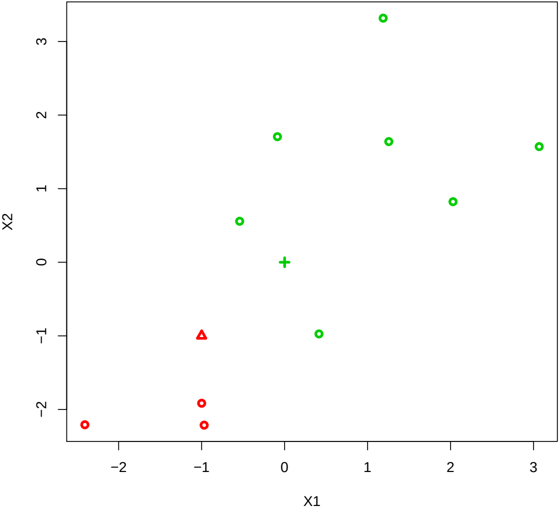
Choose mean with smaller distance:

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

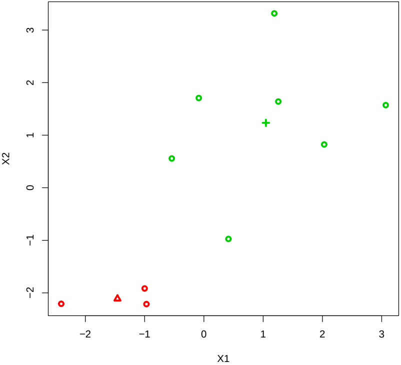
New clusters:



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

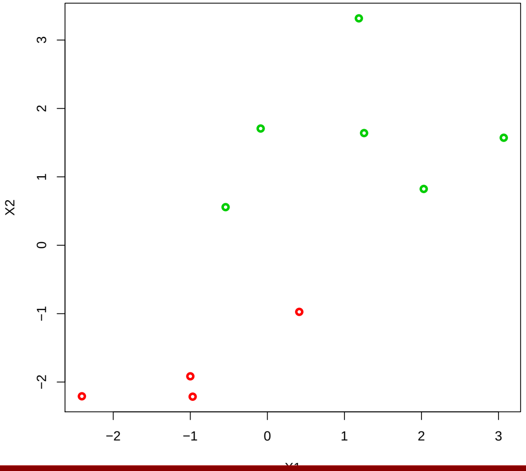
K-Means: Example

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

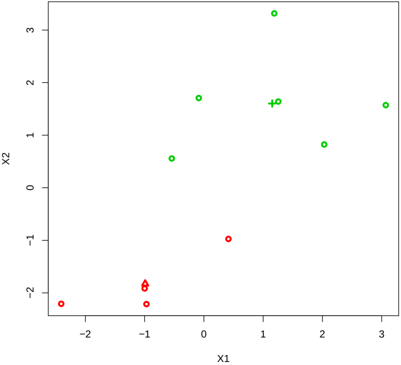
New clusters:



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

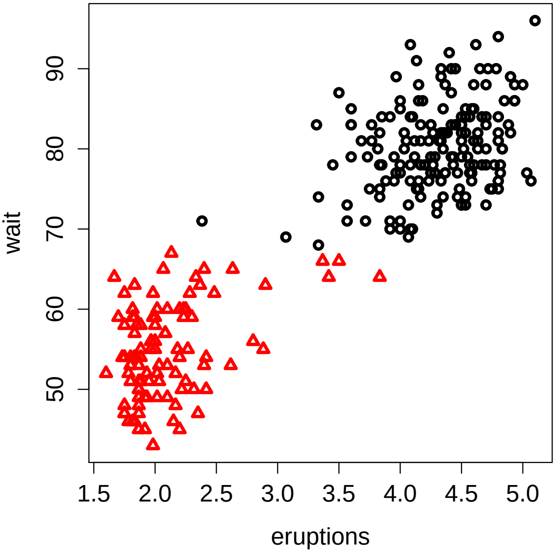
$(-1.5,-2.1)$	$(1.0,1.2)$
2.2	2.3
0.5	4.0
1.0	4.9
0.5	3.8
2.8	**1.7**
4.1	**1.2**
6.0	**2.1**
5.8	**2.0**
4.6	**0.5**
4.6	**1.1**

K-Means in Practice

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

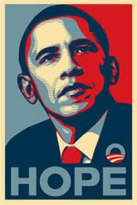
```
> library(datasets)
> faith.2 <- kmeans(faithful,2)
> names(faith.2)
> plot(faithful[,1],faithful[,2],col=faith.2$clu
 +   pch=faith.2$cluster,lwd=3)
```


wait
50
60
70
80
90
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
eruptions

K-Means in R

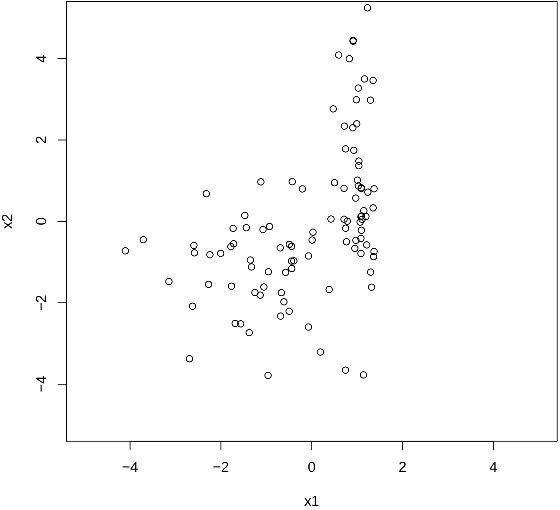
K-means can be used for *image segmentation*

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



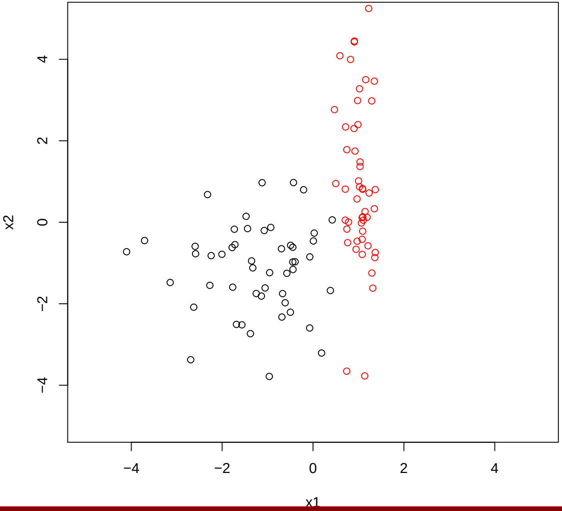
K-Means Clustering

What is our data look like this?



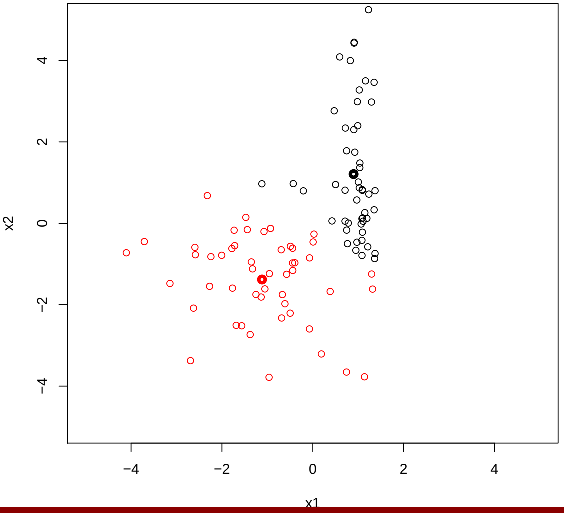
K-Means Clustering

True clustering:



K-Means Clustering

K-means clustering ($K = 2$):



Mixture Models

K-means associates data with cluster centers.

What if we actually modeled the data?

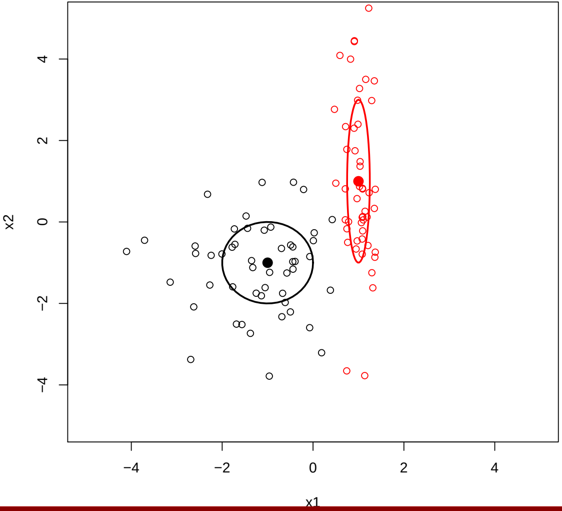
- real-valued data
- observation $\mathbf{x}_i$ in cluster c_i
- have K clusters
- model each cluster with a Gaussian distribution

$$\mathbf{x}_i \,|\, c_i = k \sim N(\mu_k, \Sigma_k)$$

- μ_k is mean vector, Σ_k is covariance matrix

Mixture Models

Gaussian mixture model ($K = 2$):



Mixture Models

Why mixture models?

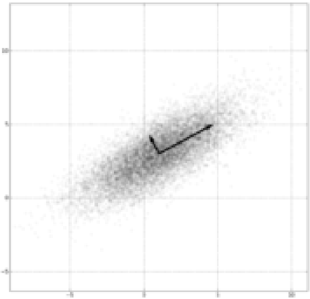
- more flexible: can account for clusters with different shapes
- have data model (will be useful for choosing K)
- less sensitive to data scaling

Multivariate Gaussian

Multivariate Gaussian distribution for $\mathbf{x} \in \mathrm{R}^d$:

$$p(\mathbf{x} \,|\, \mu, \Sigma) = (2\pi)^{-\frac{d}{2}} \, |\Sigma|^{-\frac{1}{2}} \, e^{-\frac{1}{2}(\mathbf{x}-\mu)^T \Sigma^{-1} (\mathbf{x}-\mu)}$$

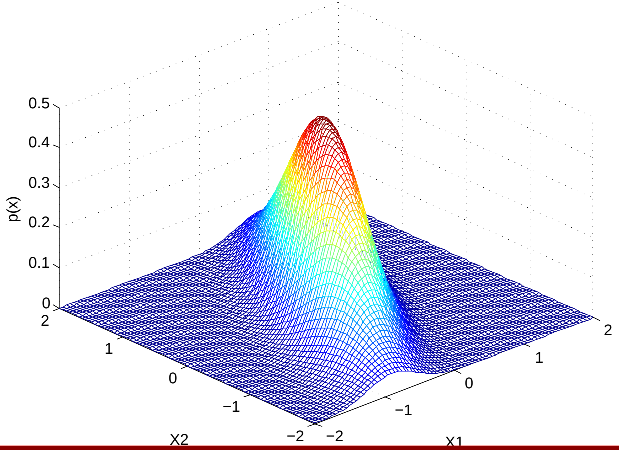
- μ is vector of means
- Σ is covariance matrix



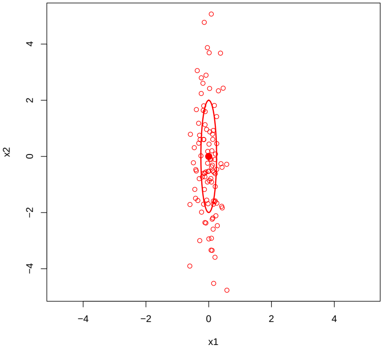
Credit: Wikipedia

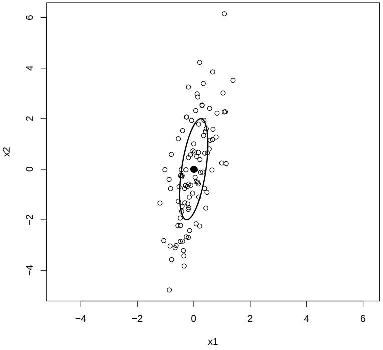
Multivariate Gaussian

pdf when $\mu = [0,0]$ and $\Sigma = \begin{bmatrix} 0.9 & 0.4 \\ 0.4 & 0.3 \end{bmatrix}$:



Multivariate Gaussian





Fitting a Mixture Model

Mixture model:

- observation $\mathbf{x}_i$ in cluster c_i with K clusters
- model each cluster with a Gaussian distribution

$$\mathbf{x}_i \,|\, c_i = k \sim N(\mu_k, \Sigma_k)$$

How do we find $c_1, \dots, c_n$ (clusters) and $(\mu_1, \Sigma_1), \dots, (\mu_K, \Sigma_K)$ (cluster centers)?

Fitting a Mixture Model

First, let’s simplify the model:

- covariance matrices have only diagonal elements,

$$\Sigma = \begin{bmatrix} \sigma_1^2 & 0 & \dots & 0 \\ 0 & \sigma_2^2 & \dots & 0 \\ \dots & \dots & \dots & 0 \\ 0 & 0 & 0 & \sigma_K^2 \end{bmatrix}$$

- set $\sigma_1^2 = \cdots = \sigma_K^2$, suppose known

Fitting a Mixture Model

Next, use a method similar to K-means:

- start with random cluster centers
- associate observations to clusters by (log-)likelihood,

$$\begin{aligned}\ell(\mathbf{x}_i \mid c_i = k) &= -\frac{d}{2}\log(2\pi) - \frac{1}{2}\log\left(\prod_{j=1}^{d}\sigma_{k,j}^2\right) - \frac{1}{2}\sum_{j=1}^{d}(x_{i,j}-\mu_{k,j})^2/\sigma_{k,j}^2 \\ &\propto -d\log(\sigma_k) - \frac{1}{2\sigma_k^2}\sum_{j=1}^{d}(x_{i,j}-\mu_{k,j})^2 \\ &\propto -\sum_{j=1}^{d}(x_{i,j}-\mu_{k,j})^2\end{aligned}$$

- refit centers $\mu_1,\ldots,\mu_K$ given clusters by

$$\mu_{k,j} = \frac{1}{n_k}\sum_{c_i=k} x_{i,j}$$

- recluster observations...

Fitting a Mixture Model

clustering with K-means

minimize distance

$$d(\mathbf{x}_i, \mu_k) = \sqrt{\sum_{j=1}^{d} (x_{i,j} - \mu_{k,j})^2}$$

clustering with GMM

maximize likelihood

$$\ell(\mathbf{x}_i \,|\, c_i = k) \propto -\sum_{j=1}^{d} (x_{i,j} - \mu_{k,j})^2$$

update means with K-means

use average

$$\mu_{k,j} = \frac{1}{n_k} \sum_{c_i = k} x_{i,j}$$

update means with GMM

use average

$$\mu_{k,j} = \frac{1}{n_k} \sum_{c_i = k} x_{i,j}$$

Fitting a Mixture Model

OK, now what if

$$\Sigma = \begin{bmatrix} \sigma_1^2 & 0 & \dots & 0 \\ 0 & \sigma_2^2 & \dots & 0 \\ \dots & \dots & \dots & 0 \\ 0 & 0 & 0 & \sigma_K^2 \end{bmatrix}$$

and $\sigma_1^2, \dots, \sigma_K^2$ can take different values?

- use same algorithm
- update μ_k and σ_k^2 with maximum likelihood estimator,

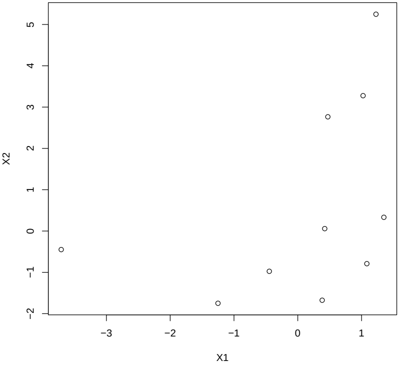
$$\mu_{k,j} = \frac{1}{n_k} \sum_{c_i = k} x_{i,j}$$

$$\sigma_{k,j}^2 = \frac{1}{n_k} \sum_{c_i = k} (x_{i,j} - \mu_{k,j})^2$$

Fitting a Mixture Model

Data:

x_1	x_2
-3.7	-0.4
0.4	0.1
0.4	-1.7
-0.4	-1.0
-1.3	-1.7
1.0	3.3
1.2	5.2
1.3	0.3
1.1	-0.8
0.5	2.8



Fitting a Mixture Model

- pick centers and variances, $\mu_1 = [-1,-1]$, $\sigma_1^2 = [1,1]$, $\mu_1 = [1,1]$, $\sigma_1^2 = [1,1]$
- compute (proportional) log likelihoods,

$$\ell(\mathbf{x}_i \,|\, c_i = k) = -\sum_{j=1}^{d} \log(\sigma_j) - \frac{1}{2}\sum_{j=1}^{d}(x_{i,j} - \mu_{k,j})^2/\sigma_{k,j}^2$$

x_1	x_2	$k = 1$	$k = 2$
-3.7	-0.4	-3.8	-12.1
0.4	0.1	-1.6	-0.6
0.4	-1.7	-1.2	-3.8
-0.4	-1.0	-0.2	-3.0
-1.3	-1.7	-0.3	-6.3
1.0	3.3	-11.2	-2.6
1.2	5.2	-22.0	-9.0
1.3	0.3	-3.6	-0.3
1.1	-0.8	-2.2	-1.6
0.5	2.8	- 8.2	-1.7

Fitting a Mixture Model

- fit new means and variances:

$$\begin{aligned}\mu_1 &= [-1.3, -1.2] \\ \sigma_1^2 &= [3.1, 0.4] \\ \mu_2 &= [0.9, 1.8] \\ \sigma_2^2 &= [0.2, 5.4]\end{aligned}$$

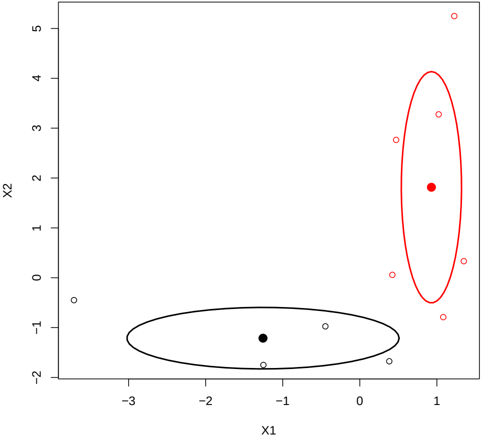
- compute new distances...

Fitting a Mixture Model

x_1	x_2	$k = 1$	$k = 2$
-3.7	-0.4	-1.8	-70.8
0.4	0.1	-2.7	-1.0
0.4	-1.7	-0.8	-2.0
-0.4	-1.0	-0.3	-6.8
-1.3	-1.7	-0.5	-16.6
1.0	3.3	-27.4	-0.1
1.2	5.2	-55.9	-1.3
1.3	0.3	-4.3	-0.7
1.1	-0.8	-1.2	-0.6
0.5	2.8	-21.3	-0.7

No change, so clusters are final

Fitting a Mixture Model



Limitations of *k*-means / mixture models

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?