Gaussian Mixture Models, Expectation Maximization

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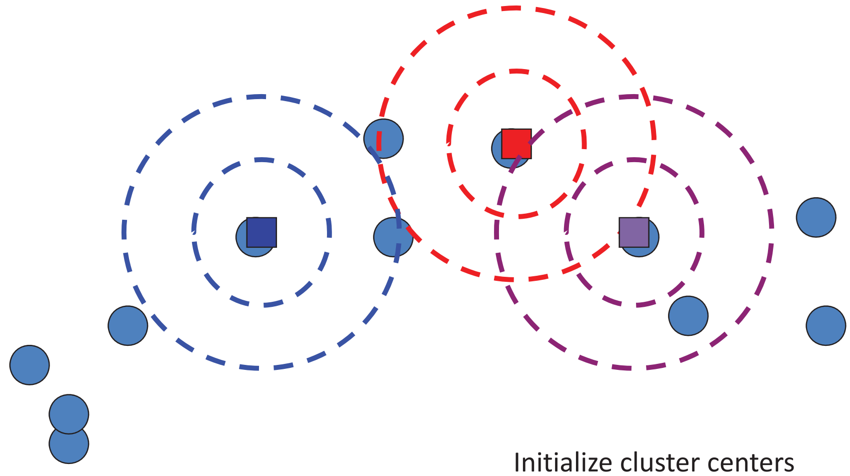
The instructor gratefully acknowledges Andrew Ng (Stanford), Andrew Moore (CMU), Eric Eaton (UPenn), David Kauchak (Pomona), and the many others who made their course materials freely available online.

Gaussian Mixture Models Overview

Learning Goals

- Describe the differences between *k*-means and GMMs

K-Means: Another View



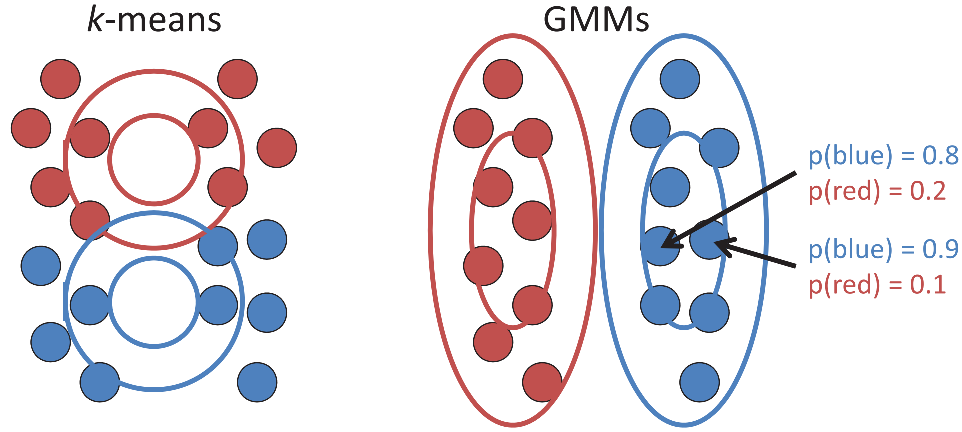
Initialize cluster centers
Assign examples to closest center
  k-means assumes spherical clusters
Update cluster centers

Based on slides by David Kauchak

Gaussian Mixture Models

- Assume data came from **mixture of Gaussians** (**elliptical data**)
- Assign data to cluster with certain **probability** (**soft clustering**)

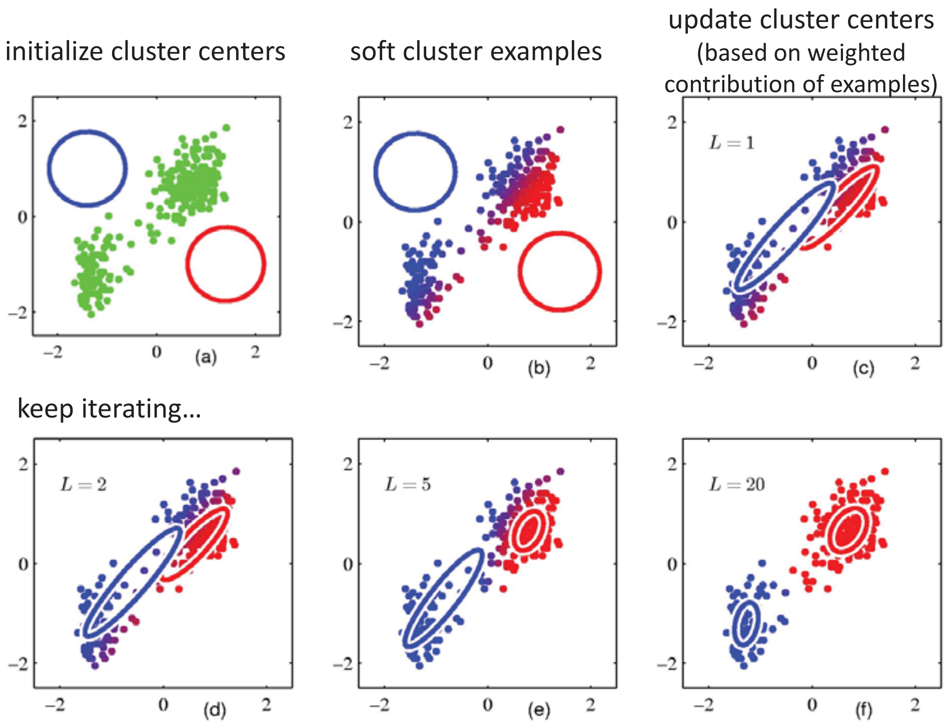
k-means GMMs



- Very similar at high-level to *k*-means: iterate between assigning examples and updating cluster centers

Based on slides by David Kauchak

GMM Example



Based on slides by David Kauchak [Images by Chris Bishop, PRML]

Learning GMMs

Learning Goals

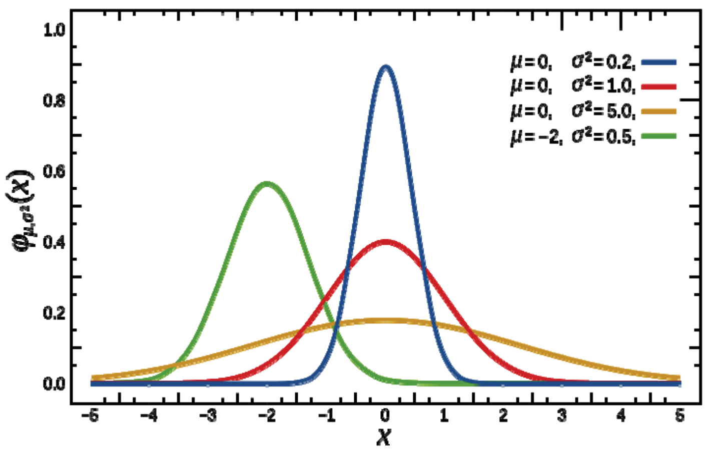
- Describe the technical details of GMMs

Univariate Gaussian Distribution

(scalar) random variable X

parameters: (scalar) mean μ, (scalar) variance σ^2

$$X \sim N(\mu, \sigma^2) \qquad p(x; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$



Wikipedia [Normal Distribution]

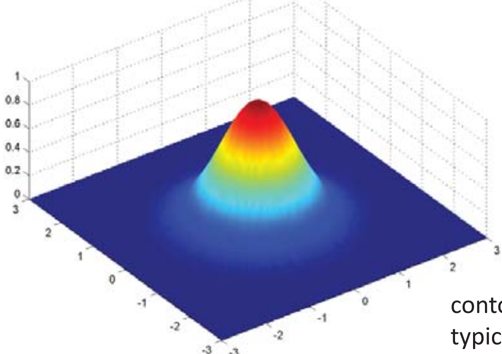
Multivariate Gaussian Distribution

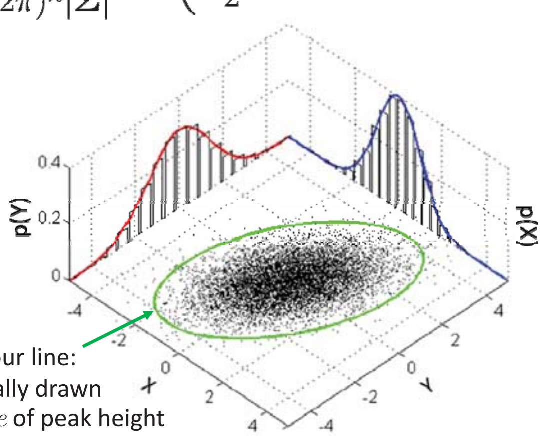
random variable vector $\boldsymbol{X} = [X_1, \ldots, X_n]^T$

parameters: mean vector $\boldsymbol{\mu} \in \mathbb{R}^n$

covariance matrix $\boldsymbol{\Sigma}$ (symmetric, positive definite)

$$\boldsymbol{X} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \qquad p(\boldsymbol{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^n |\boldsymbol{\Sigma}|}} \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x}-\boldsymbol{\mu})\right)$$





Wikipedia [Multivariate Normal Distribution]

Covariance Matrix

Recall for pair of r.v.'s X and Y, covariance is defined as

$$\mathrm{cov}(X, Y) = \mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])]$$

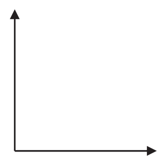
For $\boldsymbol{X} = [X_1, \ldots, X_n]^T$, **covariance matrix** summarizes covariances across all pairs of variables:

$$\boldsymbol{\Sigma} = \mathbb{E}[(\boldsymbol{X} - \mathbb{E}[\boldsymbol{X}])(\boldsymbol{X} - \mathbb{E}[\boldsymbol{X}])^T]$$

$$\boldsymbol{\Sigma} \text{ is } n \times n \text{ matrix s.t. } \Sigma_{ij} = \mathrm{cov}(X_i, X_j)$$

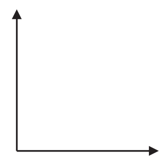
___ parameters

$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_1^2 & \sigma_{12} & \cdots & \sigma_{1n} \\ \sigma_{21} & \sigma_2^2 & \cdots & \sigma_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{n1} & \sigma_{n2} & \cdots & \sigma_n^2 \end{bmatrix}$$



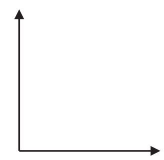
___ params

$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_1^2 & & 0 \\ & \sigma_2^2 & \\ 0 & \ddots & \sigma_n^2 \end{bmatrix}$$



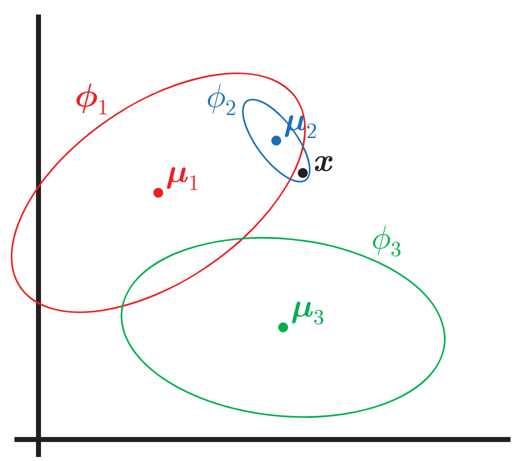
___ params

$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma^2 & & 0 \\ & \sigma^2 & \\ 0 & \ddots & \sigma^2 \end{bmatrix}$$



GMMs as Generative Model

- There are k components
- Component j
  - has associated mean vector $\boldsymbol{\mu}_j$ and covariance matrix $\boldsymbol{\Sigma}_j$
  - generates data from $N(\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$
- Each example $\boldsymbol{x}^{(i)}$ is generated according to following recipe:
  - pick component j at random with probability ϕ_j
  - sample $\boldsymbol{x}^{(i)} \sim N(\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$



GMMs as Generative Model

We are given training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(n)}\}$ (w/o labels)

We model data by specifying joint distribution

$$p(\boldsymbol{x}^{(i)}, z^{(i)}) = p(\boldsymbol{x}^{(i)}) \mid z^{(i)})\ p(z^{(i)})$$

Here, for k components,

$$z^{(i)} \sim \text{Multinomial}(\phi) \qquad \phi_j = p(z^{(i)} = j)$$

$$\phi_j \geq 0, \textstyle\sum_{j=1}^{k} \phi_j = 1$$

$$\boldsymbol{x}^{(i)} \mid z^{(i)} = j \sim N(\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$$

Goals: Determine $z^{(i)}$ (soft cluster assignments)

Determine model parameters ϕ_j, $\boldsymbol{\mu}_j$, $\boldsymbol{\Sigma}_j$ $(1 \leq j \leq k)$

Note: $z^{(i)}$ are **latent** r.v.'s (they are hidden/unobserved)

This is what makes estimation problem difficult

Based on notes by Andrew Ng

GMM Optimization

Assume supervised setting (known cluster assignments)

MLE for univariate Gaussian

$$\hat{\mu} = \frac{1}{n} \underbrace{\sum_{i=1}^{n}}_{\text{sum over points generated from this Gaussian}} x^{(i)} \qquad \hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^{n} \left(x^{(i)} - \hat{\mu}\right)^2$$

MLE for multivariate Gaussian

$$\hat{\boldsymbol{\mu}} = \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{x}^{(i)} \qquad \hat{\boldsymbol{\Sigma}} = \frac{1}{n} \sum_{i=1}^{n} \left(\boldsymbol{x}^{(i)} - \hat{\boldsymbol{\mu}}\right) \left(\boldsymbol{x}^{(i)} - \hat{\boldsymbol{\mu}}\right)^T$$

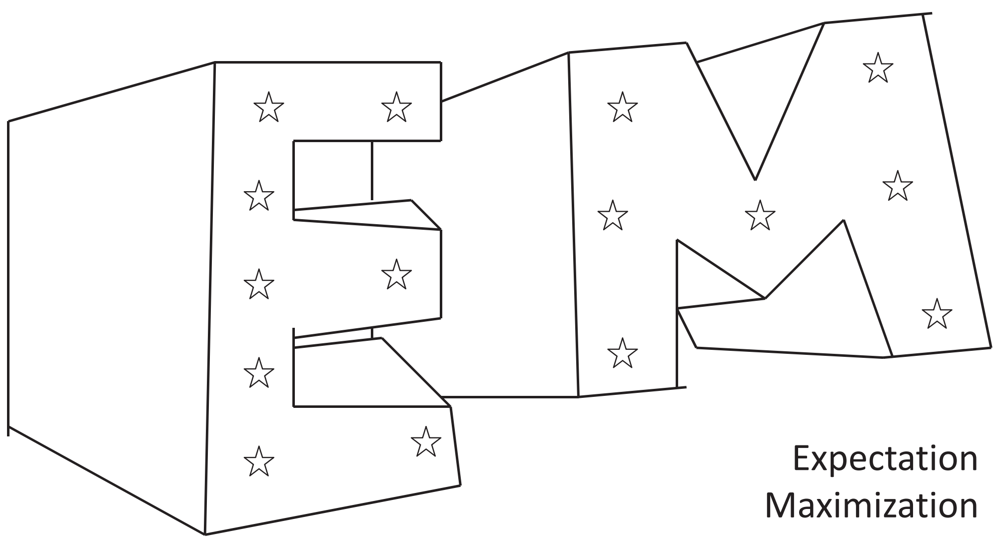
Based on slides by David Sontag

GMM Optimization

What if unobserved data?

Now what?

Based on notes by Andrew Ng



Expectation
Maximization

Based on slides by Andrew Moore

DETOUR

Expectation Maximization

Learning Goals

- Describe when EM is useful
- Describe the two steps of EM
- Practice EM on a toy problem

Expectation Maximization

- Clever method for maximizing marginal likelihoods

$$\arg\max_{\theta} \prod_{i=1}^{n} P\left(\boldsymbol{x}^{(i)}\right) = \arg\max_{\theta} \prod_{i=1}^{n} \sum_{j=1}^{k} P\left(\boldsymbol{x}^{(i)}, z^{(i)} = j\right)$$

- Excellent approach for unsupervised learning
- Can do “trivial” things (upcoming example)
- One of most general unsupervised approaches with many other uses (e.g. HMM inference)

Overview

- Begin with guess for model parameters
- Repeat until convergence
  - Update latent variables based on our expectations [E-step]
  - Update model parameters to maximize log likelihood [M-step]

Based on notes by Andrew Ng and slides by Andrew Moore

Silly Example

Let events be "grades in a class"

component 1 = gets an A P(A) = ½

component 2 = gets a B P(B) = p

component 3 = gets a C P(C) = $2p$

component 4 = gets a D P(D) = ½ $- 3p$ (note $0 \leq p \leq 1/6$)

Assume we want to estimate p from data. In a given class, there were

a A's, b B's, c C's, d D's.

What is the MLE of *p* given a, b, c, d?

so if class got

a	*b*	*c*	*d*
14	6	9	10

Same Problem with Hidden Information

Someone tells us that

# of high grades (A's + B's) = h

# of C's = c

# of D's = d

What is the MLE of p now?

Remember

P(A) = ½

P(B) = p

P(C) = $2p$

P(D) = ½ $- 3p$

We can answer this question circularly:

EXPECTATION If we know value of p, we could compute **expected** values of a and b.

MAXIMIZATION If we know expected values of a and b, we could compute **maximum** likelihood value of p.

EM for Our Silly Example

- Begin with initial guess for p
- Iterate between Expectation and Maximization to improve our estimates of p and a & b

- Define $p^{(t)}$ = estimate of p on t^{th} iteration
  $b^{(t)}$ = estimate of b on t^{th} iteration
- Repeat until convergence

E-step
$$b^{(t)} = \frac{p^{(t)}}{\frac{1}{2} + p^{(t)}} h \qquad = \mathbb{E}[b|p^{(t)}]$$

M-step
$$p^{(t+1)} = \frac{b^{(t)} + c}{6\left(b^{(t)} + c + d\right)} \qquad = \text{MLE of } p \text{ given } b^{(t)}$$

Based on slides by Andrew Moore [Clustering with Gaussian Mixtures]

EM Convergence

- Good news: converging to local optima is guaranteed
- Bad news: local optima

Aside (idea behind convergence proof)

- likelihood must increase or remain same between each iteration [not obvious]
- likelihood can never exceed 1 [obvious]
- so likelihood must converge [obvious]

In our example, suppose we had

$$h = 20,\ c = 10,\ d = 10$$
$$p^{(0)} = 0$$

Error generally decreases by constant factor each time step (e.g. convergence is linear)

t	$p^{(t)}$	$b^{(t)}$
0	0	0
1	0.0833	2.857
2	0.0937	3.158
3	0.0947	3.185
4	0.0948	3.187
5	0.0948	3.187
6	0.0948	3.187

Based on slides by Andrew Moore [Clustering with Gaussian Mixtures]

EM Applied to GMMs

Learning Goals

- Describe how to optimize GMMs using EM

Learning GMMs

Recall $\boldsymbol{z}^{(i)}$ indicates which of *k* Gaussians each $\boldsymbol{x}^{(i)}$ comes from

If $\boldsymbol{z}^{(i)}$'s were known, maximizing likelihood is easy

$$\ell(\boldsymbol{\phi}, \mu, \Sigma) = \sum_{i=1}^{n} \log P(\boldsymbol{x}^{(i)} | z^{(i)}; \boldsymbol{\phi}, \mu, \Sigma) + \log P(z^{(i)}; \boldsymbol{\phi})$$

Maximize wrt ϕ, μ, Σ gives

$$\phi_j = \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}\left[\left[z^{(i)} = j\right]\right]$$

fraction of examples assigned to component j

$$\boldsymbol{\mu}_j = \frac{\sum_{i=1}^{n} \mathbb{I}\left[\left[z^{(i)} = j\right]\right] \boldsymbol{x}^{(i)}}{\sum_{i=1}^{n} \mathbb{I}\left[\left[z^{(i)} = j\right]\right]}$$

mean and covariance of examples assigned to component j

$$\boldsymbol{\Sigma}_j = \frac{\sum_{i=1}^{n} \mathbb{I}\left[\left[z^{(i)} = j\right]\right] \left(\boldsymbol{x}^{(i)} - \boldsymbol{\mu}_j\right) \left(\boldsymbol{x}^{(i)} - \boldsymbol{\mu}_j\right)^T}{\sum_{i=1}^{n} \mathbb{I}\left[\left[z^{(i)} = j\right]\right]}$$

Based on notes by Andrew Ng

Learning GMMs

Since $z^{(i)}$'s are not known, use EM!

Repeat until convergence
[E-step] Know model parameters, "guess" values of $z^{(i)}$'s

[M-step] Know class probabilities, update model parameters

Based on notes by Andrew Ng

(This slide intentionally left blank.)

Learning GMMs

Since $z^{(i)}$'s are not known, use EM!

compare to k-means
$w_j^{(i)} \to c^{(i)} = \delta(z^{(i)} = j \mid x^{(i)}; \boldsymbol{\phi}, \mu, \Sigma)$
"hard" assignment to nearest cluster

Repeat until convergence

[E-step] Know model parameters, "guess" values of $z^{(i)}$'s

for each i,j, set

$$w_j^{(i)} = p(z^{(i)} = j | \boldsymbol{x}^{(i)}; \boldsymbol{\phi}, \boldsymbol{\mu}, \Sigma)$$

$w_j^{(i)}$'s are "soft" guesses for values of $z^{(i)}$'s

compute posterior probability using Bayes' Rule

$$= \frac{\boxed{p\left(\boldsymbol{x}^{(i)} | z^{(i)} = j; \boldsymbol{\mu}, \Sigma\right)} \boxed{p\left(z^{(i)} = j; \boldsymbol{\phi}\right)}}{\sum_{l=1}^{k} p\left(\boldsymbol{x}^{(i)} | z^{(i)} = l; \boldsymbol{\mu}, \Sigma\right) p\left(z^{(i)} = l; \boldsymbol{\phi}\right)}$$

evaluate Gaussian w/ μ_j & Σ_j at $\boldsymbol{x}^{(i)}$

prior probability of being assigned to component $j = \phi_j$

[M-step] Know class probabilities, update model parameters

update parameters

$$\phi_j = \frac{1}{n} \sum_{i=1}^{n} w_j^{(i)} \qquad \boldsymbol{\mu}_j = \frac{\sum_{i=1}^{n} w_j^{(i)} \boldsymbol{x}^{(i)}}{\sum_{i=1}^{n} w_j^{(i)}}$$

$$\boldsymbol{\Sigma}_j = \frac{\sum_{i=1}^{n} w_j^{(i)} \left(\boldsymbol{x}^{(i)} - \boldsymbol{\mu}_j\right) \left(\boldsymbol{x}^{(i)} - \boldsymbol{\mu}_j\right)^T}{\sum_{i=1}^{n} w_j^{(i)}}$$

same equations as when $z^{(i)}$'s are known except $\mathbb{I}[[z^{(i)} = j]]$ replaced with probability $w_j^{(i)}$

Based on notes by Andrew Ng

Final Comments

EM is not magic

- Still optimizing non-convex function with lots of local optima
- Computations are just easier (often, significantly so!)

Problems

- EM susceptible to local optima

$\Rightarrow$ reinitialize at several different initial parameters

Extensions

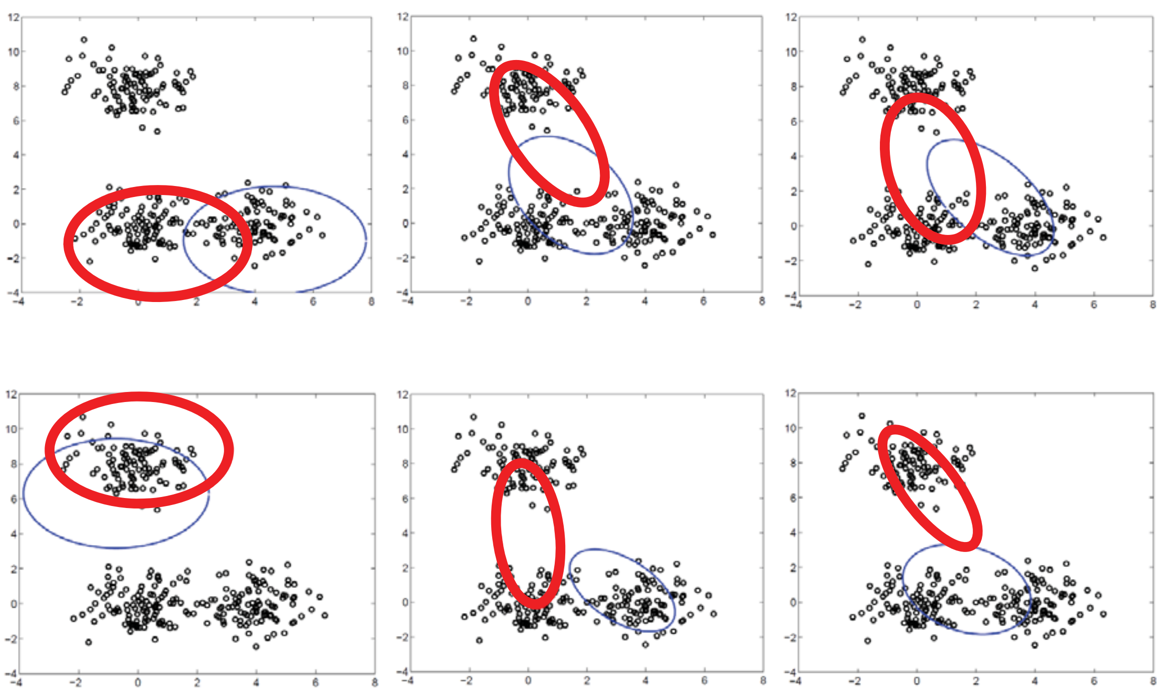
- EM looks at maximum log likelihood of data

$\Rightarrow$also possible to look at maximum *a posteriori*

GMM Exercise

We estimated a mixture of two Gaussians based on two-dimensional data shown below. The mixture was initialized randomly in two different ways and run for three iterations based on each initialization. However, the figures got mixed up. Please draw an arrow from one figure to another to indicate how they follow from each other (you should only draw *four* arrows).

Exercise by Tommi Jaakola



Exercise by Tommi Jaakola