Clustering with Gaussian Mixtures

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CSG220
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Adapted from the Andrew Moore tutorial of the same name

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Unsupervised Learning

- You walk into a bar.
  A stranger approaches and tells you:
  "I've got data from k classes. Each class produces observations with a normal distribution and variance $\sigma^2 I$. Standard simple multivariate gaussian assumptions. I can tell you the probabilities of each class ."
- So far, looks straightforward.
  "I need a maximum likelihood estimate of the μ_i's ."
- "No problem," you think.
  "There's just one thing. None of the data are labeled. I have datapoints, but I don't know what class they're from (any of them!)
- Uh oh!!

Multivariate Gaussian Density

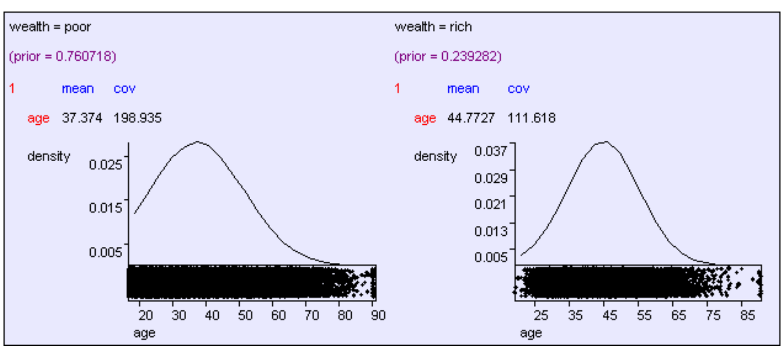
$$p(\mathbf{x}) = \frac{1}{(2\pi)^{m/2} \, || \, \boldsymbol{\Sigma} \, ||^{1/2}} \exp\left[-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma} (\mathbf{x} - \boldsymbol{\mu}) \right]$$

where

$\boldsymbol{\mu}$ = mean (m - dimensional vector)

$\boldsymbol{\Sigma}$ = covariance ($m \times m$ matrix)

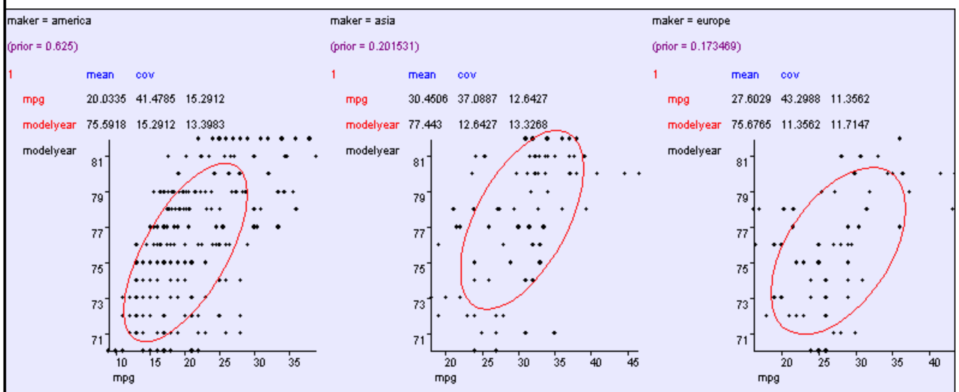
Predicting wealth from age



1-dimensional Gaussians

General: *O(m²)* parameters

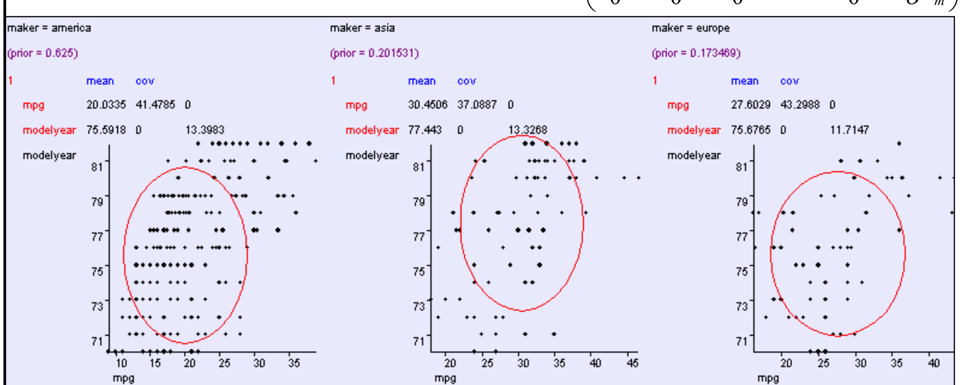
$$\Sigma = \begin{pmatrix} \sigma^2{}_1 & \sigma_{12} & \cdots & \sigma_{1m} \\ \sigma_{12} & \sigma^2{}_2 & \cdots & \sigma_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{1m} & \sigma_{2m} & \cdots & \sigma^2{}_m \end{pmatrix}$$



2-dimensional Gaussians

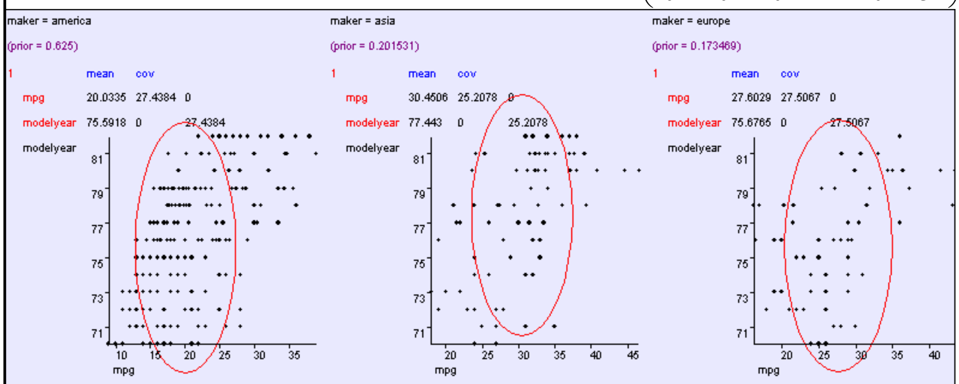
Aligned: *O(m)* parameters

$$\Sigma = \begin{pmatrix} \sigma^2{}_1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \sigma^2{}_2 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \sigma^2{}_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \sigma^2{}_{m-1} & 0 \\ 0 & 0 & 0 & \cdots & 0 & \sigma^2{}_m \end{pmatrix}$$



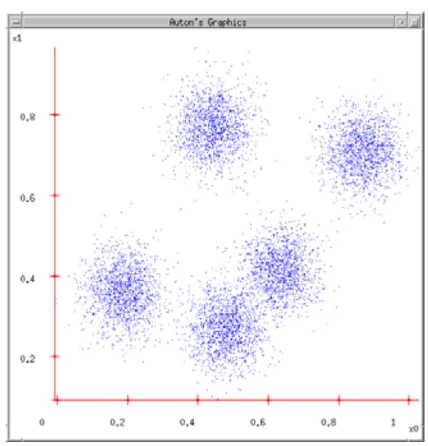
Spherical: *O(1)* cov parameters

$$\Sigma = \begin{pmatrix} \sigma^2 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \sigma^2 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \sigma^2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \sigma^2 & 0 \\ 0 & 0 & 0 & \cdots & 0 & \sigma^2 \end{pmatrix}$$



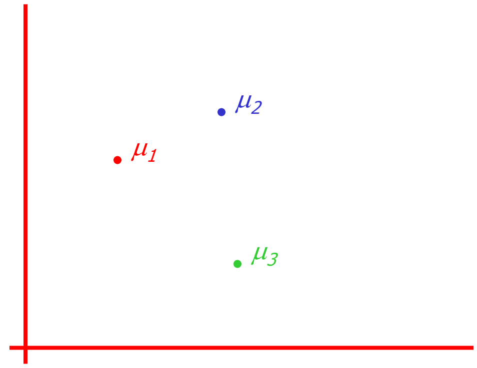
What if we want to do density estimation with multimodal or clumpy data?

Clearly not modeled well by a single Gaussian



The Gaussian Mixture Model assumption

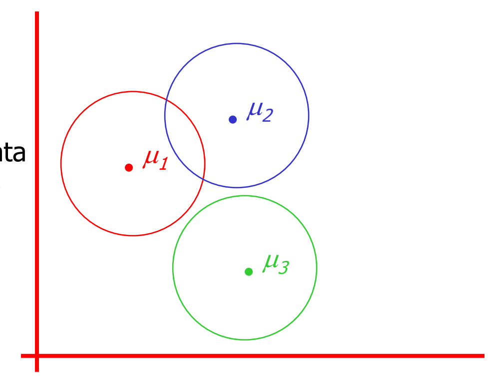
- There are k components. The i'th component is called ω_i
- Component ω_i has an associated mean vector μ_i



The Gaussian Mixture Model assumption

- There are k components. The i'th component is called ω_i
- Component ω_i has an associated mean vector μ_i
- Each component generates data from a Gaussian with mean μ_i and covariance matrix $\sigma^2\boldsymbol{I}$

Assume that each datapoint is generated according to the following recipe:



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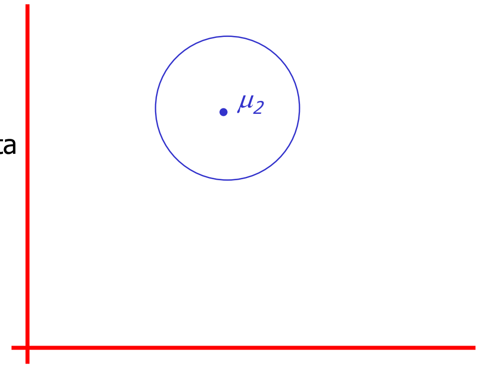
1. Pick a component at random. Choose component i with probability $P(\omega_i)$.



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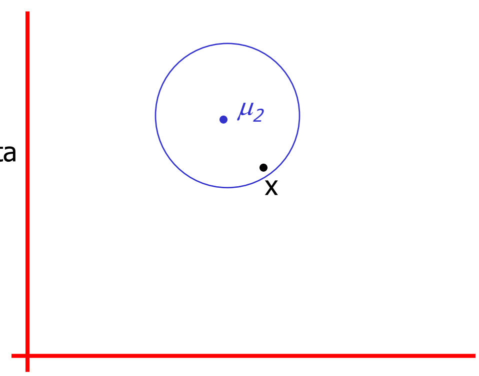
Assume that each datapoint is generated according to the following recipe:

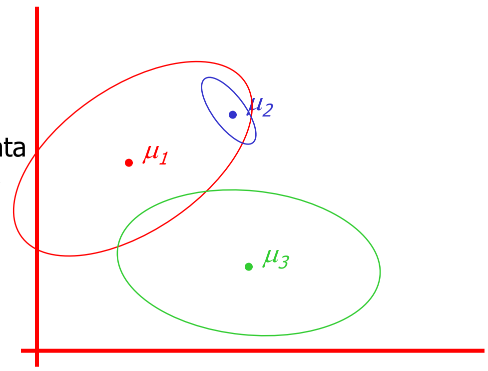
1. Pick a component at random. Choose component i with probability $P(\omega_i)$.
2. Datapoint ~ N(μ_i, $\sigma^2 \boldsymbol{I}$)

Denotes Gaussian with given mean and covariance



The General GMM assumption

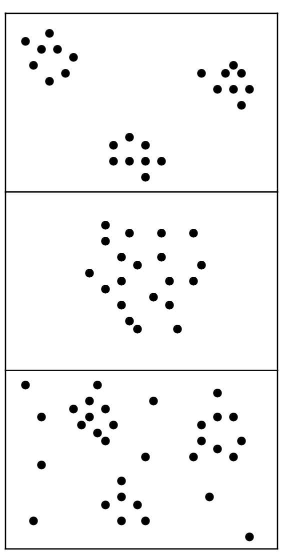
- There are k components. The i'th component is called ω_i
- Component ω_i has an associated mean vector μ_i
- Each component generates data from a Gaussian with mean μ_i and covariance matrix Σ_i



Assume that each datapoint is generated according to the following recipe:

1. Pick a component at random. Choose component i with probability $P(\omega_i)$.
2. Datapoint ~ N(μ_i, Σ_i)

Unsupervised Learning: not as hard as it looks



Sometimes easy

Sometimes impossible

and sometimes in between

*IN CASE YOU'RE WONDERING WHAT THESE DIAGRAMS ARE, THEY SHOW 2-d UNLABELED DATA (**X** VECTORS) DISTRIBUTED IN 2-d SPACE. THE TOP ONE HAS THREE VERY CLEAR GAUSSIAN CENTERS*

Computing likelihoods in unsupervised case

We have $\boldsymbol{x}_1 , \boldsymbol{x}_2 , \ldots \boldsymbol{x}_R$

We know $P(\omega_1)\ P(\omega_2)\ ..\ P(\omega_k)$

We know σ

$p(\boldsymbol{x}|\ \omega_i, \boldsymbol{\mu}_i, \ldots \boldsymbol{\mu}_k)$ = Prob density that an observation from class ω_i would have value $\boldsymbol{x}$ given class means $\boldsymbol{\mu}_1 \ldots \boldsymbol{\mu}_k$

Can we write an expression for that?

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Can we write an expression for that?

Yes: The standard multivariate Gaussian using mean $\boldsymbol{\mu}_i$

likelihoods in unsupervised case

We have $x_{1,} x_2 \ldots x_R$
We have $P(\omega_1)$, ..., $P(\omega_k)$. We have σ.
We can define, for any x , $p(x| \omega_i , \mu_1, \mu_2 .. \mu_k)$

Can we define $p(x \mid \mu_1, \mu_2 .. \mu_k)$?

Can we define $p(x_1, x_1, .. x_n \mid \mu_1, \mu_2 .. \mu_k)$?

likelihoods in unsupervised case

We have $x_{1,} x_2 \ldots x_R$
We have $P(\omega_1)$, ..., $P(\omega_k)$. We have σ.
We can define, for any x , $p(x| \omega_i , \mu_1, \mu_2 .. \mu_k)$

Can we define $p(x \mid \mu_1, \mu_2 .. \mu_k)$?

Yes: A weighted sum of multivariate Gaussians,
where the weighting of the i^{th} component is $P(\omega_i)$

Can we define $p(x_1, x_1, .. x_n \mid \mu_1, \mu_2 .. \mu_k)$?

Yes, if we assume the x's were drawn independently

Unsupervised Learning: Mediumly Good News

We now have a procedure s.t. if you give me a guess at $\mu_1, \mu_2 .. \mu_k,$

I can tell you the prob of the unlabeled data given those μ's.

(From Duda and Hart)

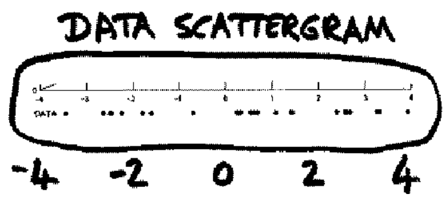
Suppose x's are 1-dimensional.

There are two classes; ω_1 and ω_2

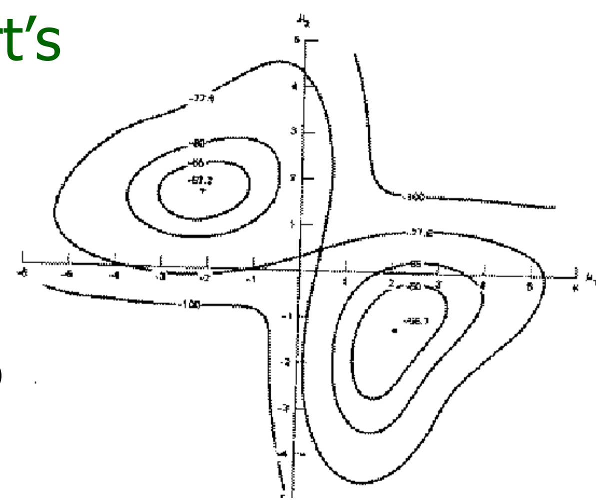
$P(\omega_1) = 1/3$ $P(\omega_2) = 2/3$ $\sigma = 1$.

There are 25 unlabeled datapoints

$x_1 = 0.608$
$x_2 = -1.590$
$x_3 = 0.235$
$x_4 = 3.949$
:
$x_{25} = -0.712$



Duda & Hart's Example



Graph of
log p($x_1, x_2 .. x_{25} \mid \mu_1, \mu_2$)
against μ_1(→) and μ_2(↑)

Max likelihood = (μ_1 =-2.13, μ_2 =1.668)

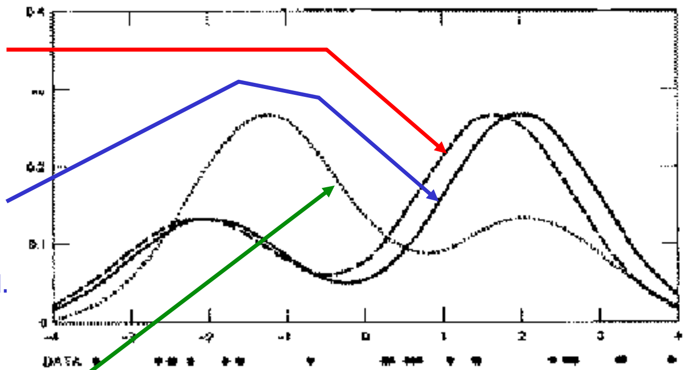
Local maximum, but very close to global at (μ_1 =2.085, μ_2 =-1.257)*

* corresponds to switching ω_1 and ω_2.

Duda & Hart's Example

We can graph the prob. dist. function of data given our μ_1 and μ_2 estimates.

We can also graph the true function from which the data was randomly generated.



- They are close. Good.
- The 2nd solution tries to put the "2/3" hump where the "1/3" hump should go, and vice versa.
- In this example unsupervised is almost as good as supervised. If the x_1 .. x_{25} are given the class which was used to learn them, then the results are (μ_1=-2.176, μ_2=1.684). Unsupervised got (μ_1=-2.13, μ_2=1.668).

Finding the max likelihood $\mu_1, \mu_2 .. \mu_k$

We can compute P(data | $\mu_1, \mu_2 .. \mu_k$)

How do we find the μ_i's which give max. likelihood?

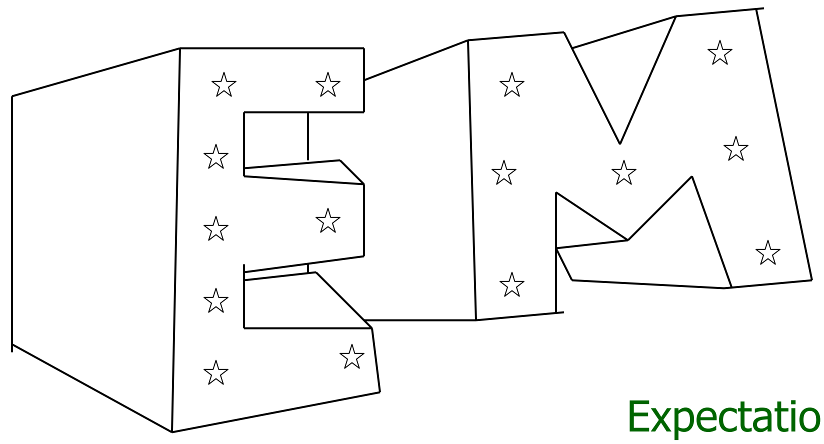
- The normal max likelihood trick:

  Set $\frac{\partial}{\partial \mu_i}$ log Prob (….) = 0

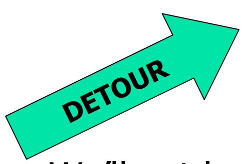
  and solve for μ_i's.

  # Here you get non-linear non-analytically-solvable equations
- Use gradient descent

  Slow but doable
- Use a much faster, cuter, and recently very popular method…



Expectation
Maximization



The E.M. Algorithm

- We'll get back to unsupervised learning soon.
- But now we'll look at an even simpler case with hidden information.
- The EM algorithm
  - Can do trivial things, such as the contents of the next few slides.
  - An excellent way of doing our unsupervised learning problem, as we'll see.
  - Many, many other uses, including inference of Hidden Markov Models.

Silly Example

Let events be "grades in a class"

w_1 = Gets an A	P(A) = ½
w_2 = Gets a B	P(B) = μ
w_3 = Gets a C	P(C) = 2μ
w_4 = Gets a D	P(D) = ½-3μ

(Note $0 \le \mu \le 1/6$)

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

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

What's the maximum likelihood estimate of μ given a,b,c,d ?

Trivial Statistics

P(A) = ½ P(B) = μ P(C) = 2μ P(D) = ½-3μ

$P(a,b,c,d \mid \mu) = K(½)^a(\mu)^b(2\mu)^c(½-3\mu)^d$

$\log P(a,b,c,d \mid \mu) = \log K + a\log ½ + b\log \mu + c\log 2\mu + d\log (½-3\mu)$

$$\text{FOR MAX LIKE } \mu\text{, SET } \frac{\partial \log P}{\partial \mu} = 0$$

$$\frac{\partial \log P}{\partial \mu} = \frac{b}{\mu} + \frac{2c}{2\mu} - \frac{3d}{1/2 - 3\mu} = 0$$

$$\text{Gives max like } \mu = \frac{b+c}{6(b+c+d)}$$

So if class got

A	B	C	D
14	6	9	10

$$\text{Max like } \mu = \frac{1}{10}$$

Boring, but true!

Same Problem with Hidden Information

Someone tells us that

Number of High grades (A's + B's) = *h*

Number of C's = *c*

Number of D's = *d*

What is the max. like estimate of μ now?

REMEMBER
P(A) = ½
P(B) = μ
P(C) = 2μ
P(D) = ½-3μ

Same Problem with Hidden Information

Someone tells us that

Number of High grades (A's + B's) = *h*

Number of C's = *c*

Number of D's = *d*

What is the max. like estimate of μ now?

REMEMBER
P(A) = ½
P(B) = μ
P(C) = 2μ
P(D) = ½-3μ

We can answer this question circularly:

EXPECTATION

If we know the value of μ we could compute the expected value of *a* and *b*

Since the ratio a:b should be the same as the ratio ½ : μ

$$a = \frac{1/2}{1/2 + \mu} h \qquad b = \frac{\mu}{1/2 + \mu} h$$

MAXIMIZATION

If we know the true values of *a* and *b* we could compute the maximum likelihood value of μ

$$\mu = \frac{b + c}{6(b + c + d)}$$

E.M. for our Trivial Problem

REMEMBER
P(A) = ½
P(B) = μ
P(C) = 2μ
P(D) = ½-3μ

We begin with a guess for μ

We iterate between EXPECTATION and MAXIMIZATION to improve our estimates of μ and *a* and *b*.

Define μ(t) the estimate of μ on the t'th iteration
b(t) the estimate of *b* on t'th iteration

$$\mu(0) = \text{initial guess}$$

$$b(t) = \frac{\mu(t) h}{\frac{1}{2} + \mu(t)} = \mathrm{E}[b \mid \mu(t)]$$

E-step

$$\mu(t+1) = \frac{b(t) + c}{6(b(t) + c + d)}$$

$$= \text{max like est of } \mu \text{ given } b(t)$$

M-step

Continue iterating until converged.
Good news: Converging to local optimum is assured.
Bad news: I said "local" optimum.

E.M. Convergence

- Convergence proof based on fact that Prob(data | μ) must increase or remain same between each iteration [NOT OBVIOUS]
- But it can never exceed 1 [OBVIOUS]

So it must therefore converge [OBVIOUS]

In our example, suppose we had
h = 20
c = 10
d = 10
μ(0) = 0

t	μ(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

Convergence is generally <u>linear</u>: error decreases by a constant factor each time step.

Back to Unsupervised Learning of Gaussian Mixture Models

Remember:

We have unlabeled data x_1 x_2 … x_R
We know there are k classes
We know $P(\omega_1)$ $P(\omega_2)$ $P(\omega_3)$ … $P(\omega_k)$
We <u>don't</u> know $\boldsymbol{\mu}_1$ $\boldsymbol{\mu}_2$ .. $\boldsymbol{\mu}_k$

We can write p(data | $\boldsymbol{\mu}_1$…. $\boldsymbol{\mu}_k$)

$$= \mathrm{p}(\mathbf{x}_1 \ldots \mathbf{x}_R | \mu_1 \ldots \mu_k)$$

$$= \prod_{i=1}^{R} \mathrm{p}(\mathbf{x}_i | \mu_1 \ldots \mu_k)$$

$$= \prod_{i=1}^{R} \sum_{j=1}^{k} \mathrm{p}(\mathbf{x}_i | \omega_j, \mu_1 \ldots \mu_k) \mathrm{P}(\omega_j)$$

$$= \prod_{i=1}^{R} \sum_{j=1}^{k} \mathrm{K} \exp\left(-\frac{1}{2\sigma^2} \|\mathbf{x}_i - \mu_j\|^2\right) \mathrm{P}(\omega_j)$$

E.M. for GMMs

For Max likelihood we know $\frac{\partial}{\partial \mu_i} \log \Pr ob(\text{data} | \mu_1 \ldots \mu_k) = 0$

Some wild'n'crazy algebra turns this into : "For Max likelihood, for each j,

$$\mu_j = \frac{\sum_{i=1}^{R} P(\omega_j | \mathbf{x}_i, \mu_1 \ldots \mu_k) \mathbf{x}_i}{\sum_{i=1}^{R} P(\omega_j | \mathbf{x}_i, \mu_1 \ldots \mu_k)}$$

This is n nonlinear equations in $\boldsymbol{\mu}_j$'s."

If, for each $\mathbf{x}_i$ we knew that for each ω_j the prob that $\mathbf{x}_i$ was in class ω_j is $P(\omega_j|x_i,\mu_1\ldots\mu_k)$ … then we could easily compute $\boldsymbol{\mu}_j$.

If we knew each μ_j then we could easily compute $P(\omega_j|\mathbf{x}_i,\mu_1\ldots\mu_j)$ for each ω_j and $\mathbf{x}_i$.

…I feel an EM experience coming on!!

E.M. for GMMs

Iterate. On the *t*'th iteration let our estimates be

$$\lambda_t = \{ \mu_1(t), \mu_2(t) \ldots \mu_c(t) \}$$

E-step

Compute "expected" classes of all datapoints for each class

Just evaluate a Gaussian at x_k

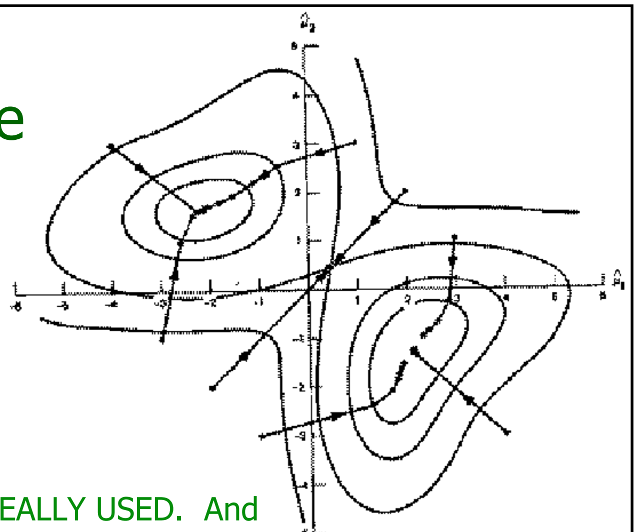
$$P(\omega_i|\mathbf{x}_k,\lambda_t) = \frac{p(\mathbf{x}_k|\omega_i,\lambda_t)P(\omega_i|\lambda_t)}{p(\mathbf{x}_k|\lambda_t)} = \frac{p(\mathbf{x}_k|\omega_i,\boldsymbol{\mu}_i(t),\sigma^2\mathbf{I})p_i(t)}{\sum_{j=1}^{c} p(\mathbf{x}_k|\omega_j,\boldsymbol{\mu}_j(t),\sigma^2\mathbf{I})p_j(t)}$$

M-step.

Compute Max. like $\boldsymbol{\mu}$ given our data's class membership distributions

$$\mu_i(t+1) = \frac{\sum_k P(\omega_i|\mathbf{x}_k,\lambda_t)\mathbf{x}_k}{\sum_k P(\omega_i|\mathbf{x}_k,\lambda_t)}$$

E.M. Convergence



- As with all EM procedures, convergence to a local optimum guaranteed.

- This algorithm is REALLY USED. And in high dimensional state spaces, too. E.G. Vector Quantization for Speech Data

E.M. for General GMMs

Iterate. On the *t*'th iteration let our estimates be

$$\lambda_t = \{ \mu_1(t), \mu_2(t) \ldots \mu_c(t), \Sigma_1(t), \Sigma_2(t) \ldots \Sigma_c(t), p_1(t), p_2(t) \ldots p_c(t) \}$$

$p_i(t)$ is shorthand for estimate of *$P(\omega_i)$* on t'th iteration

E-step

Compute "expected" classes of all datapoints for each class

$$P(\omega_i | x_k, \lambda_t) = \frac{p(\mathbf{x}_k | \omega_i, \lambda_t) P(\omega_i | \lambda_t)}{p(\mathbf{x}_k | \lambda_t)} = \frac{p(\mathbf{x}_k | \omega_i, \boldsymbol{\mu}_i(t), \boldsymbol{\Sigma}_i(t)) p_i(t)}{\sum_{j=1}^{c} p(\mathbf{x}_k | \omega_j, \boldsymbol{\mu}_j(t), \boldsymbol{\Sigma}_j(t)) p_j(t)}$$

Just evaluate a Gaussian at x_k

M-step.

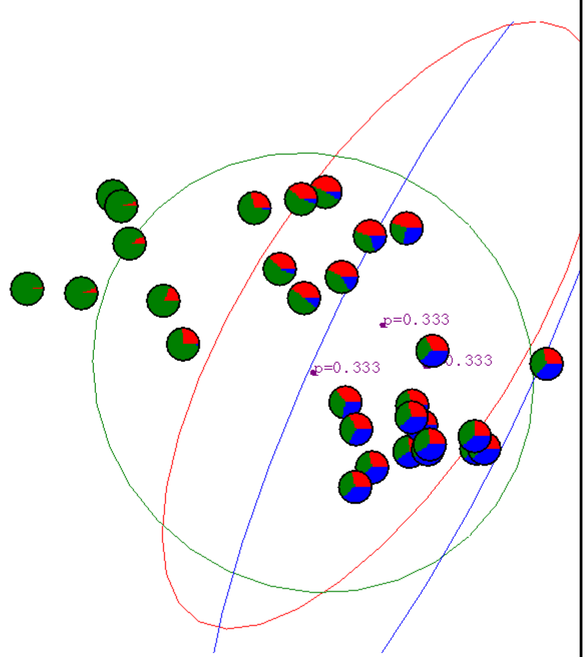
Compute Max. like **μ** given our data's class membership distributions

$$\mu_i(t+1) = \frac{\sum_k P(\omega_i | \mathbf{x}_k, \lambda_t) \mathbf{x}_k}{\sum_k P(\omega_i | \mathbf{x}_k, \lambda_t)} \qquad \boldsymbol{\Sigma}_i(t+1) = \frac{\sum_k P(\omega_i | \mathbf{x}_k, \lambda_t) [\mathbf{x}_k - \boldsymbol{\mu}_i(t+1)][\mathbf{x}_k - \boldsymbol{\mu}_i(t+1)]^T}{\sum_k P(\omega_i | \mathbf{x}_k, \lambda_t)}$$

$$p_i(t+1) = \frac{\sum_k P(\omega_i | \mathbf{x}_k, \lambda_t)}{R}$$

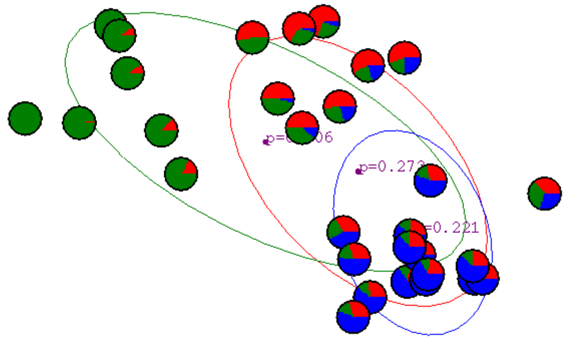
R = #records

Gaussian Mixture Example: Start

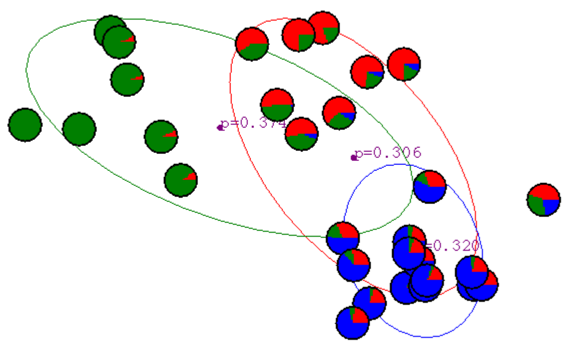


Advance apologies: in Black and White this example will be incomprehensible

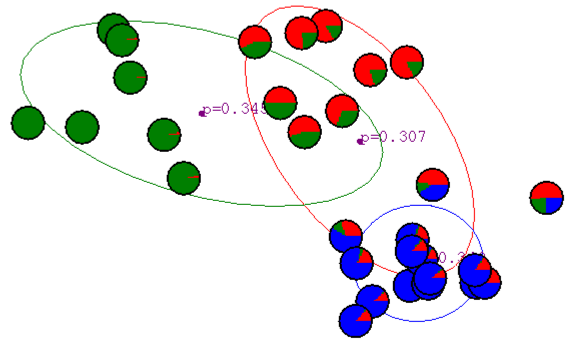
After first iteration



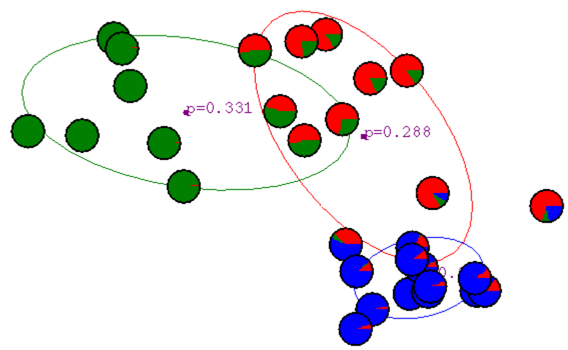
After 2nd iteration



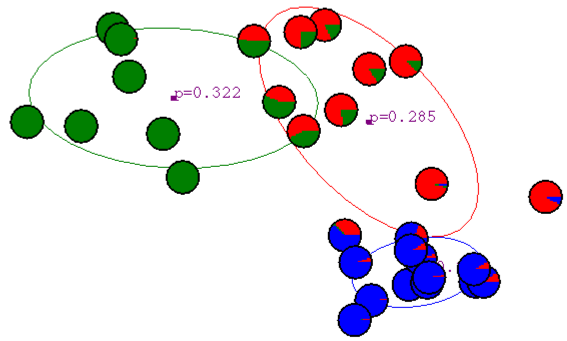
After 3rd iteration



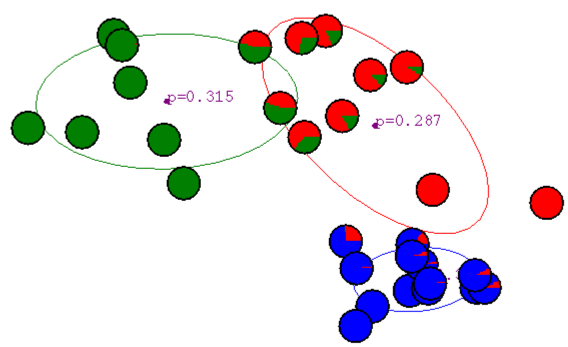
After 4th iteration



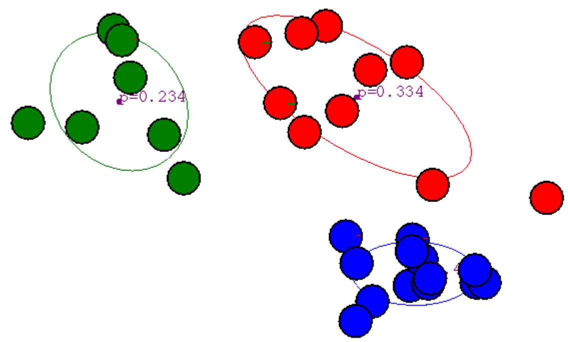
After 5th iteration



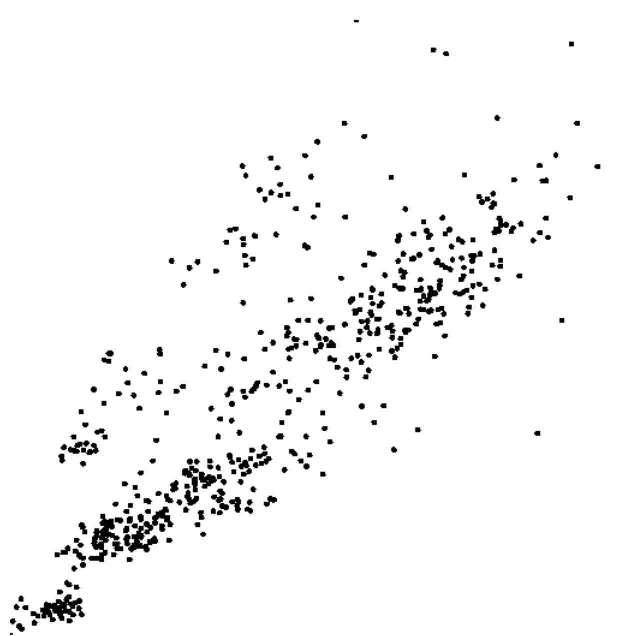
After 6th iteration



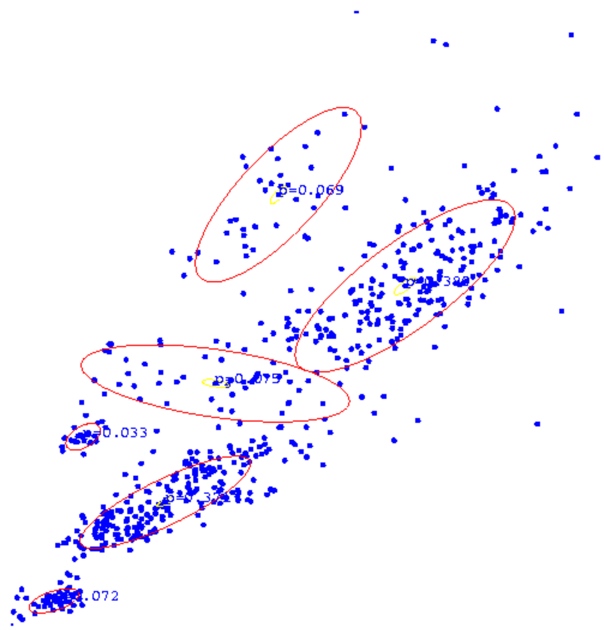
After 20th iteration



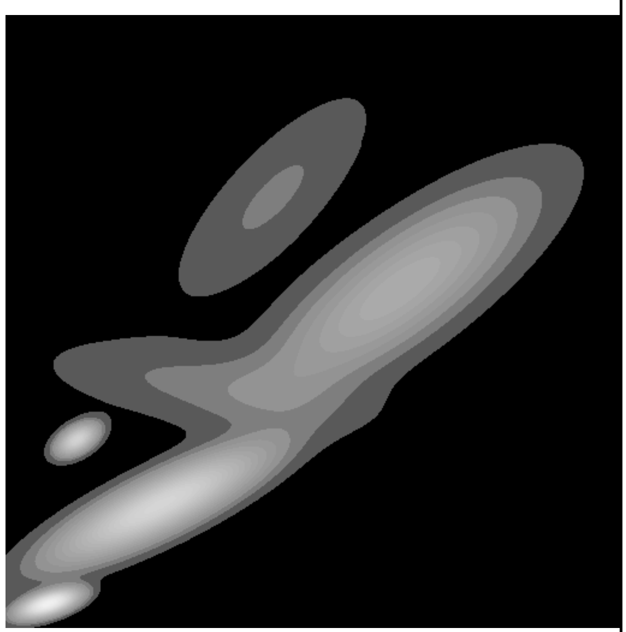
Some Bio Assay data



GMM clustering of the assay data



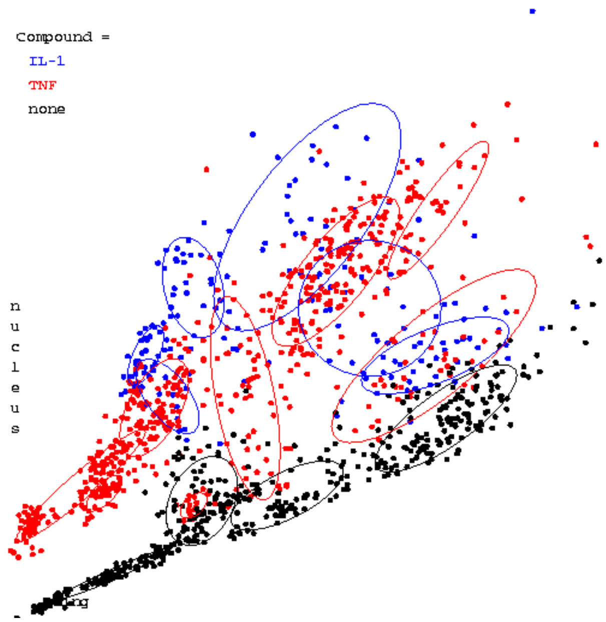
Resulting Density Estimator



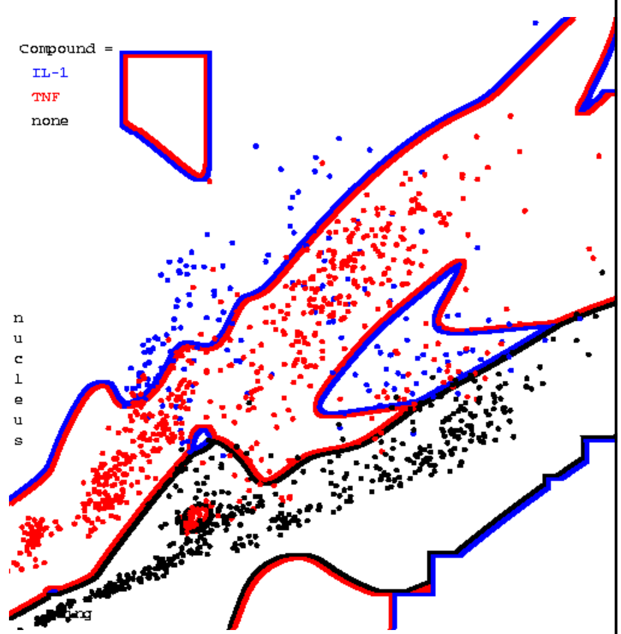
Three classes of assay

(each learned with it's own mixture model)

(Sorry, this will again be semi-useless in black and white)



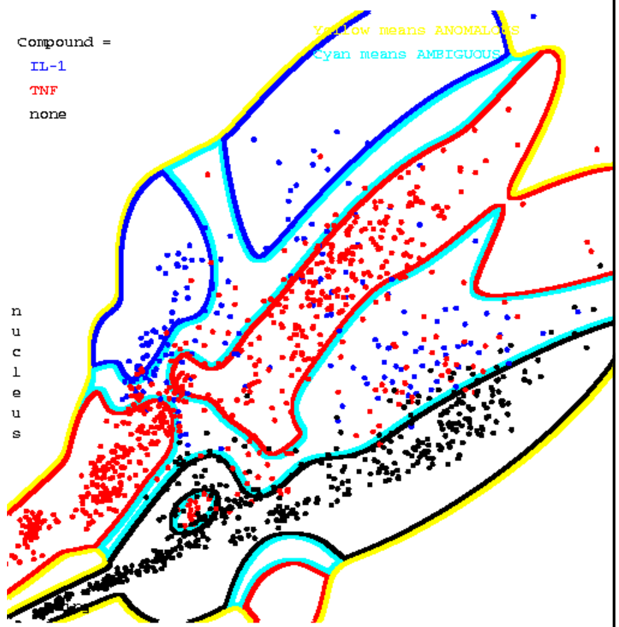
Resulting Bayes Classifier



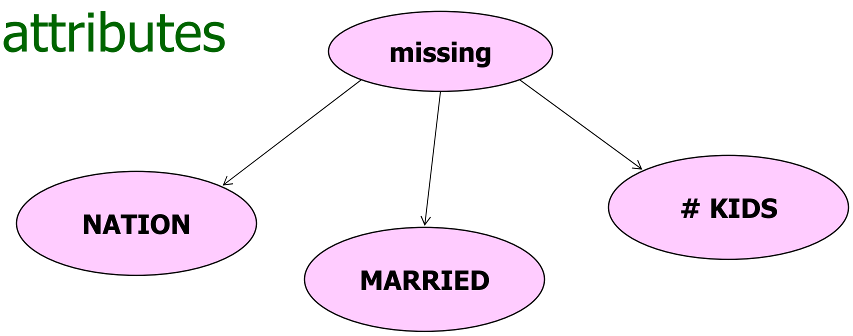
Resulting Bayes Classifier, using posterior probabilities to alert about ambiguity and anomalousness

Yellow means anomalous

Cyan means ambiguous



Unsupervised learning with symbolic attributes



It's just a "learning Bayes net with known structure but hidden values" problem.

Can use Gradient Descent.

<u>EASY</u>, fun exercise to do an EM formulation for this case too.

Final Comments

- Remember, E.M. can get stuck in local minima, and empirically it DOES.
- Our unsupervised learning example assumed $P(\omega_i)$'s known. Easy to relax this.
- It's possible to do Bayesian unsupervised learning instead of max. likelihood.
- There are other algorithms for unsupervised learning. We'll visit K-means soon. Hierarchical clustering is also interesting.
- Neural-net algorithms called "competitive learning" turn out to have interesting parallels with the EM method we saw.

What you should know

- How to "learn" maximum likelihood parameters (locally max. like.) in the case of unlabeled data.
- Be happy with this kind of probabilistic analysis.
- Understand the two examples of E.M. given in these notes.

Other unsupervised learning methods

- K-means (see next lecture)
- Hierarchical clustering (e.g. Minimum spanning trees)
- Principal Component Analysis
  - simple, useful tool
- Non-linear PCA
  - Neural Auto-Associators
  - Locally weighted PCA
  - Others…