CSE 312
Autumn 2013

The Expectation-Maximization Algorithm
(for a Two-Component Gaussian Mixture)

A Hat Trick

Two slips of paper in a hat:

Pink: $\mu = 3$, and

Blue: $\mu = 7$.

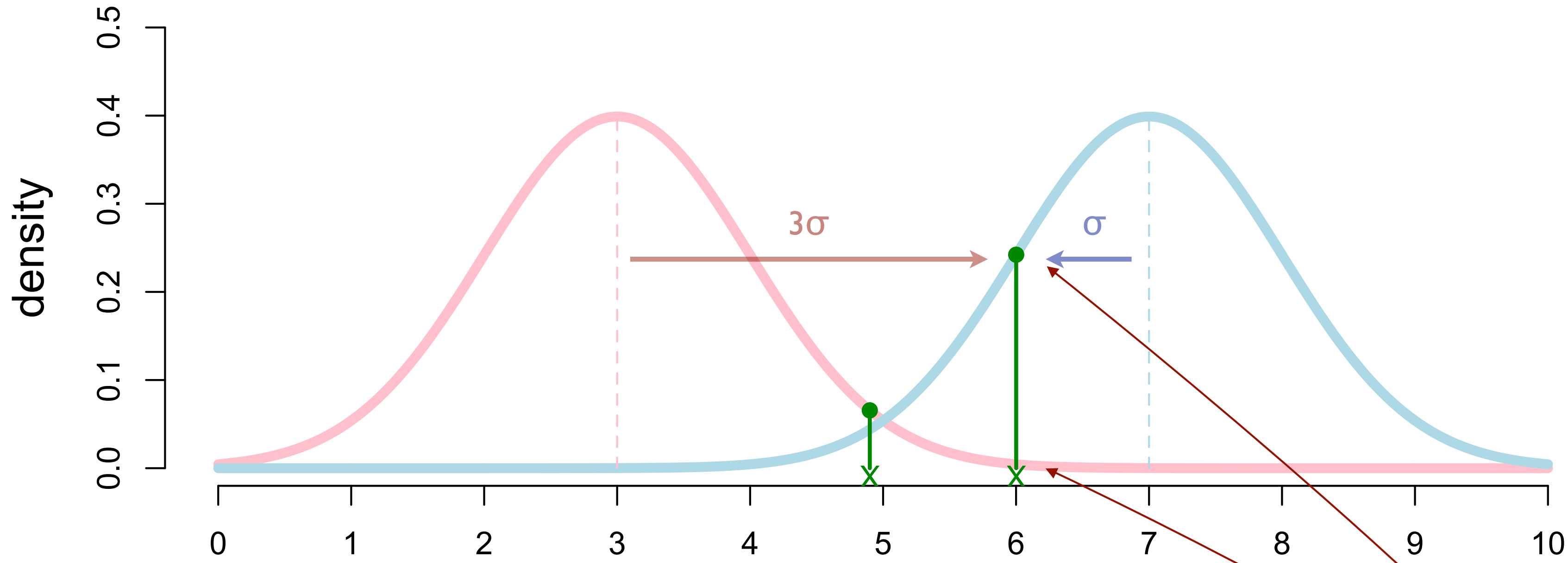
You draw one, then (without revealing color or μ) reveal a single sample $X \sim \text{Normal}(\text{mean } \mu, \sigma^2 = 1)$.

You happen to draw $X = 6.001$.

Dr. D. says “your slip = 7.” What is P(correct)?

What if X had been 4.9?

A Hat Trick



Let "$X \approx 6$" be a shorthand for $6.001 - \delta/2 < X < 6.001 + \delta/2$

$$P(\mu = 7|X = 6) = \lim_{\delta \to 0} P(\mu = 7|X \approx 6)$$

$$P(\mu = 7|X \approx 6) = \frac{P(X \approx 6|\mu = 7)P(\mu = 7)}{P(X \approx 6)}$$

Bayes rule

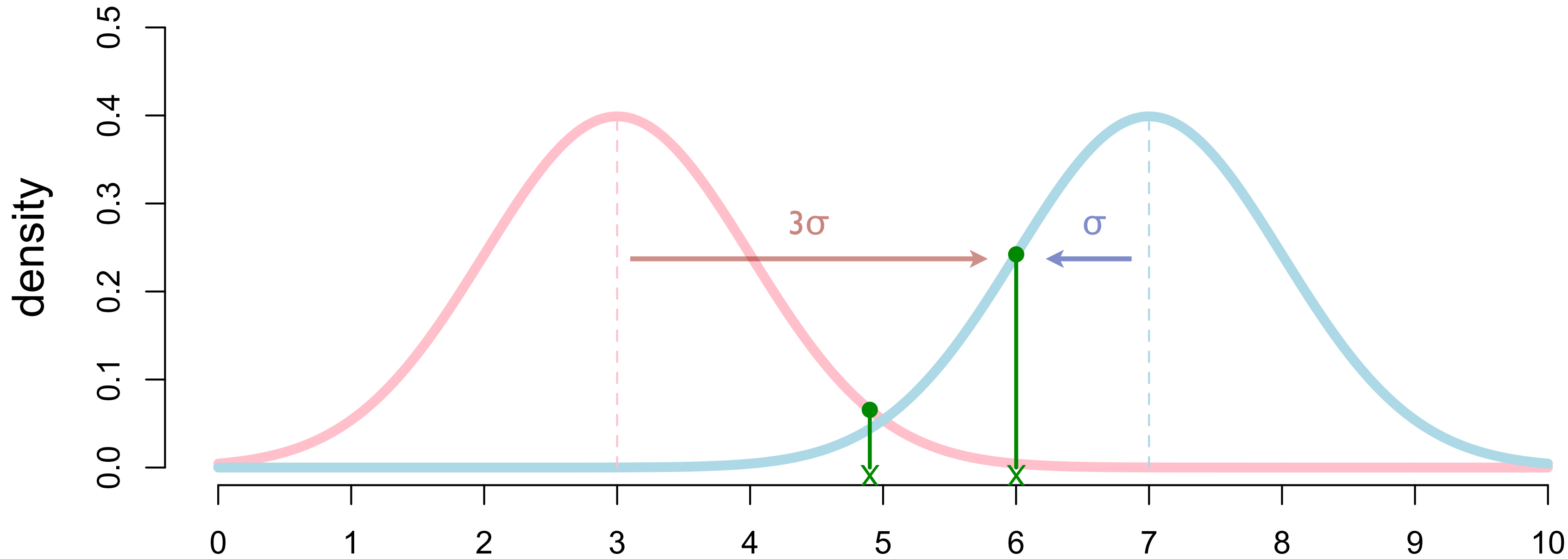
$$= \frac{0.5P(X \approx 6|\mu = 7)}{0.5P(X \approx 6|\mu = 3) + 0.5P(X \approx 6|\mu = 7)}$$

$$\approx \frac{f(X = 6|\mu = 7)\delta}{f(X = 6|\mu = 3)\delta + f(X = 6)|\mu = 7)\delta}, \text{ so}$$

$$P(\mu = 7|X = 6) = \frac{f(X = 6|\mu = 7)}{f(X = 6|\mu = 3) + f(X = 6)|\mu = 7)} \approx 0.982$$

f = normal density

A Hat Trick



Alternate View:

f = normal density

Posterior odds = Bayes Factor · Prior odds

$$\frac{P(\mu = 7 | X = 6)}{P(\mu = 3 | X = 6)} = \frac{f(X = 6 | \mu = 7)}{f(X = 6 | \mu = 3)} \cdot \frac{0.50}{0.50} = \frac{0.2422}{0.0044} \cdot \frac{1}{1} = \frac{54.8}{1}$$

I.e., 50:50 prior odds become 54:1 in favor of μ=7, given X=6.001

(and would become 3:2 in favor of μ=3, given X=4.9)

Another Hat Trick

Two secret numbers, μ_{pink} and μ_{blue}

On pink slips, many samples of Normal(μ_{pink}, $\sigma 2 = 1$),

Ditto on blue slips, from Normal(μ_{blue}, $\sigma 2 = 1$).

Based on 16 of each, how would you "guess" the secrets (where "success" means your guess is within ±0.5 of each secret)?

Roughly how likely is it that you will succeed?

Another Hat Trick (cont.)

Pink/blue = red herrings; separate & independent

Given $X_1, \ldots, X_{16} \sim N(\mu, \sigma^2)$, $\sigma^2 = 1$

Calculate $Y = (X_1 + \ldots + X_{16})/16 \sim N(? , ?)$

$E[Y] = \mu$

$Var(Y) = 16\sigma^2/16^2 = \sigma^2/16 = 1/16$

I.e., X_i's are all $\sim N(\mu, 1)$; Y is $\sim N(\mu, 1/16)$

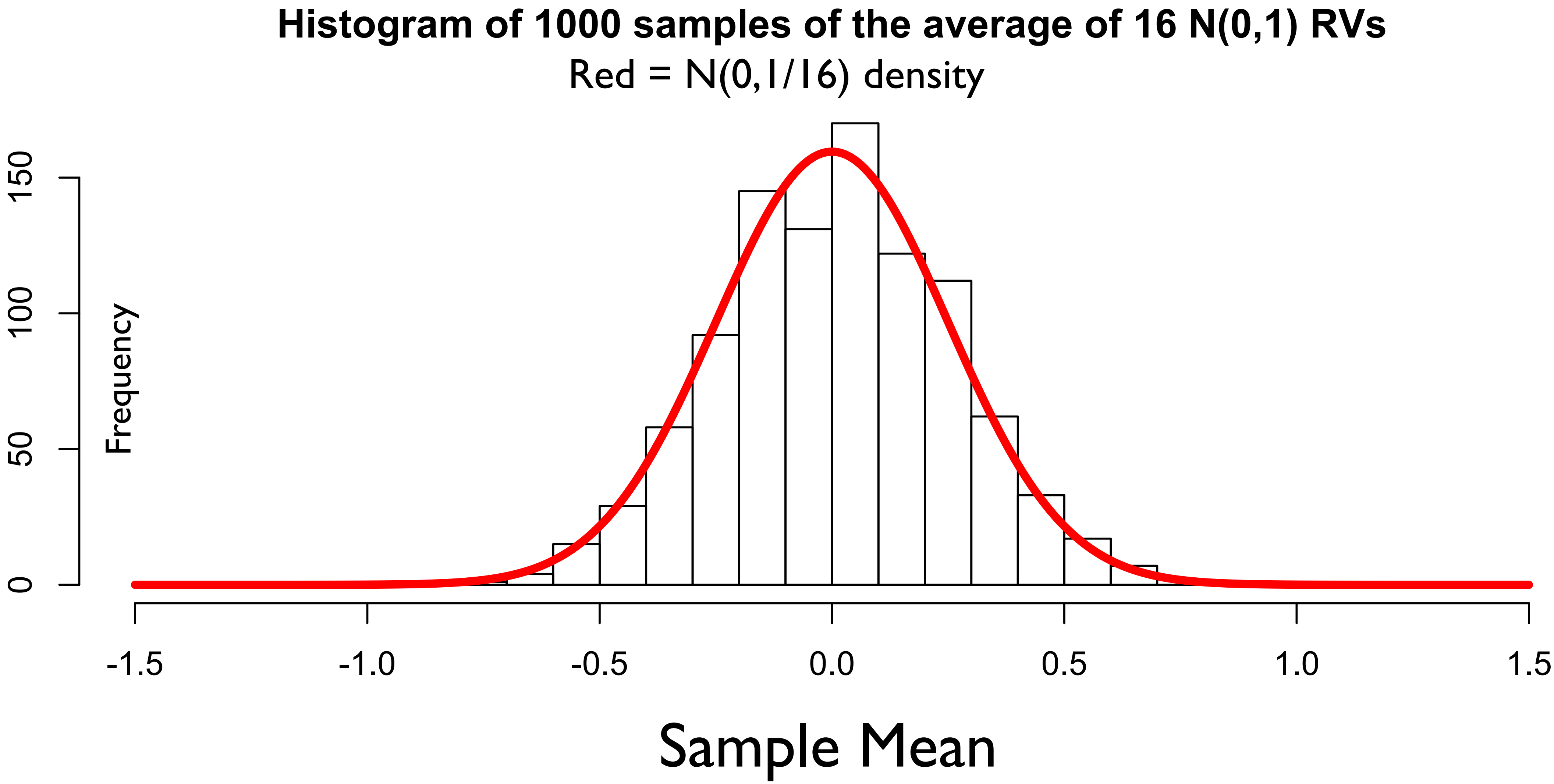
and since $0.5 = 2\ \mathrm{sqrt}(1/16)$, we have:

"Y within $\pm.5$ of μ" = "Y within $\pm 2\ \sigma$ of μ" $\approx$ 95% prob

Note 1: Y is a *point estimate* for μ;

$Y \pm 2\ \sigma$ is a *95% confidence interval* for μ

(More on this topic later)

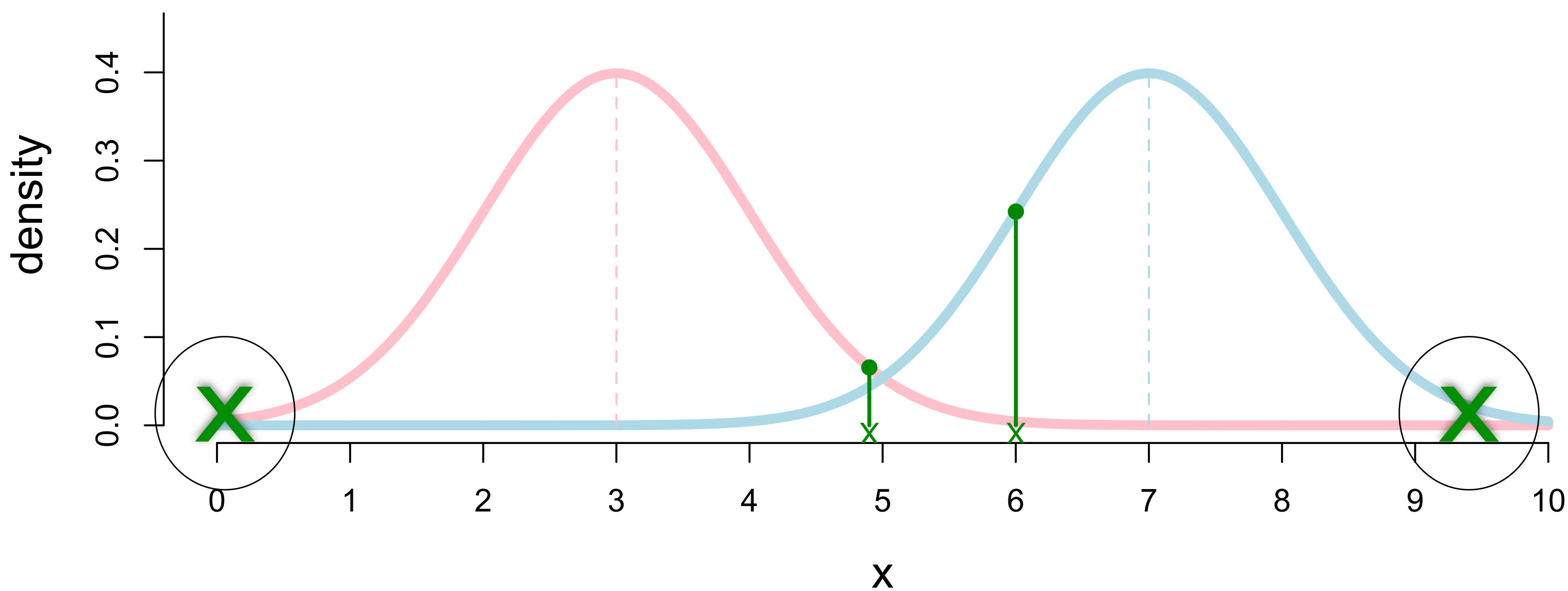

Histogram of 1000 samples of the average of 16 N(0,1) RVs
Red = N(0,1/16) density
Frequency
0
50
100
150
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
Sample Mean

Hat Trick 2 (cont.)

Note 2:

What would you do if some of the slips you pulled had coffee spilled on them, obscuring color?

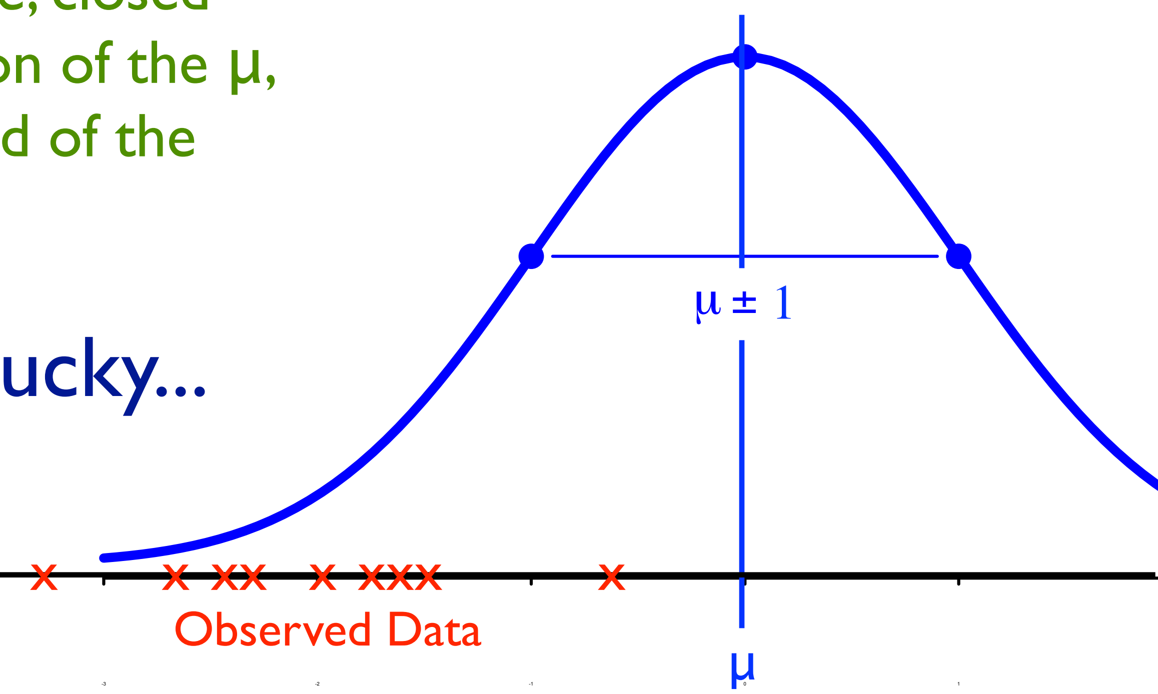
> If they were half way between means of the others?
> If they were on opposite sides of the means of the others



Previously:
How to estimate μ given data

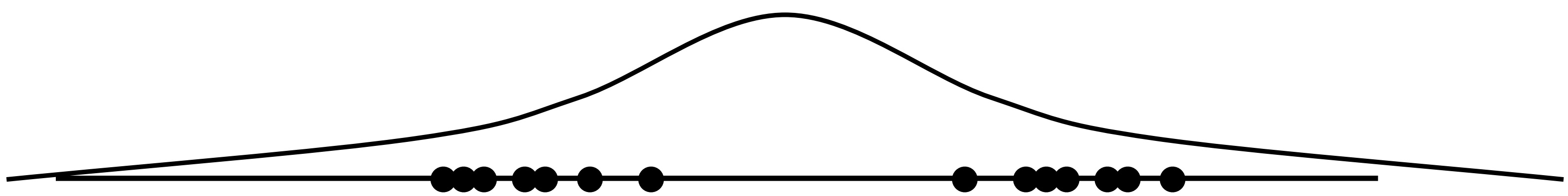
For this problem, we got a nice, closed form, solution, allowing calculation of the μ, σ that maximize the likelihood of the observed data.

We're not always so lucky...

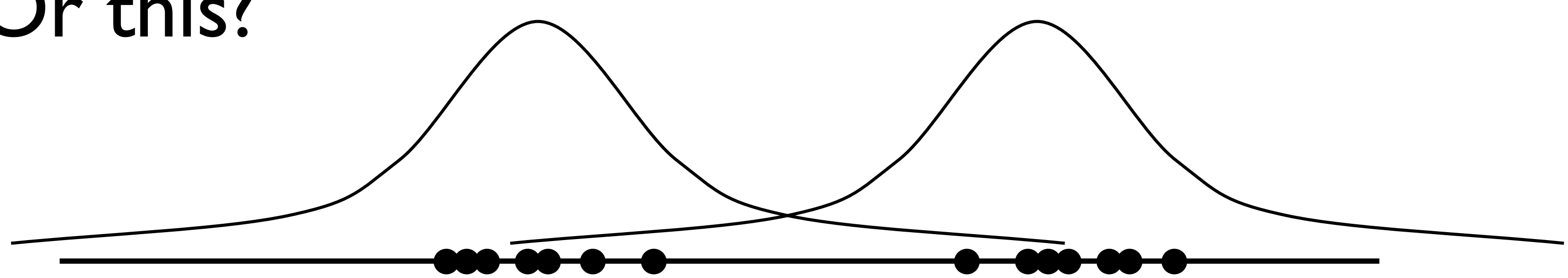


More Complex Example

This?

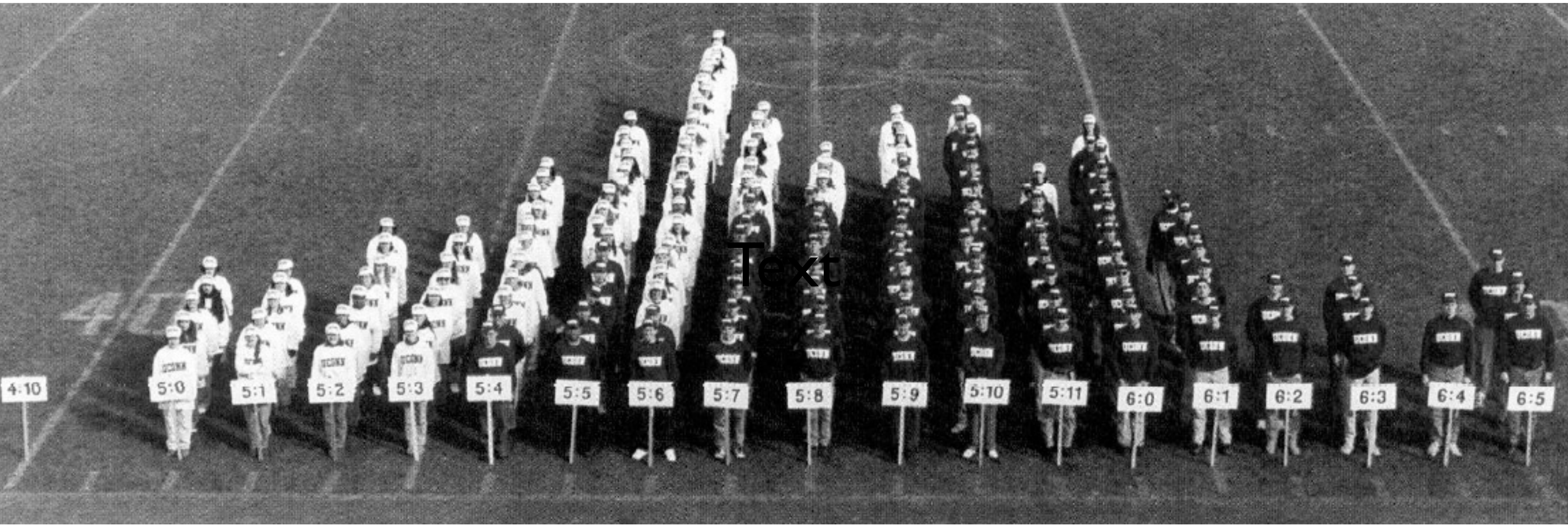


Or this?



(A modeling decision, not a math problem...,
but if the later, what math?)

A Living Histogram

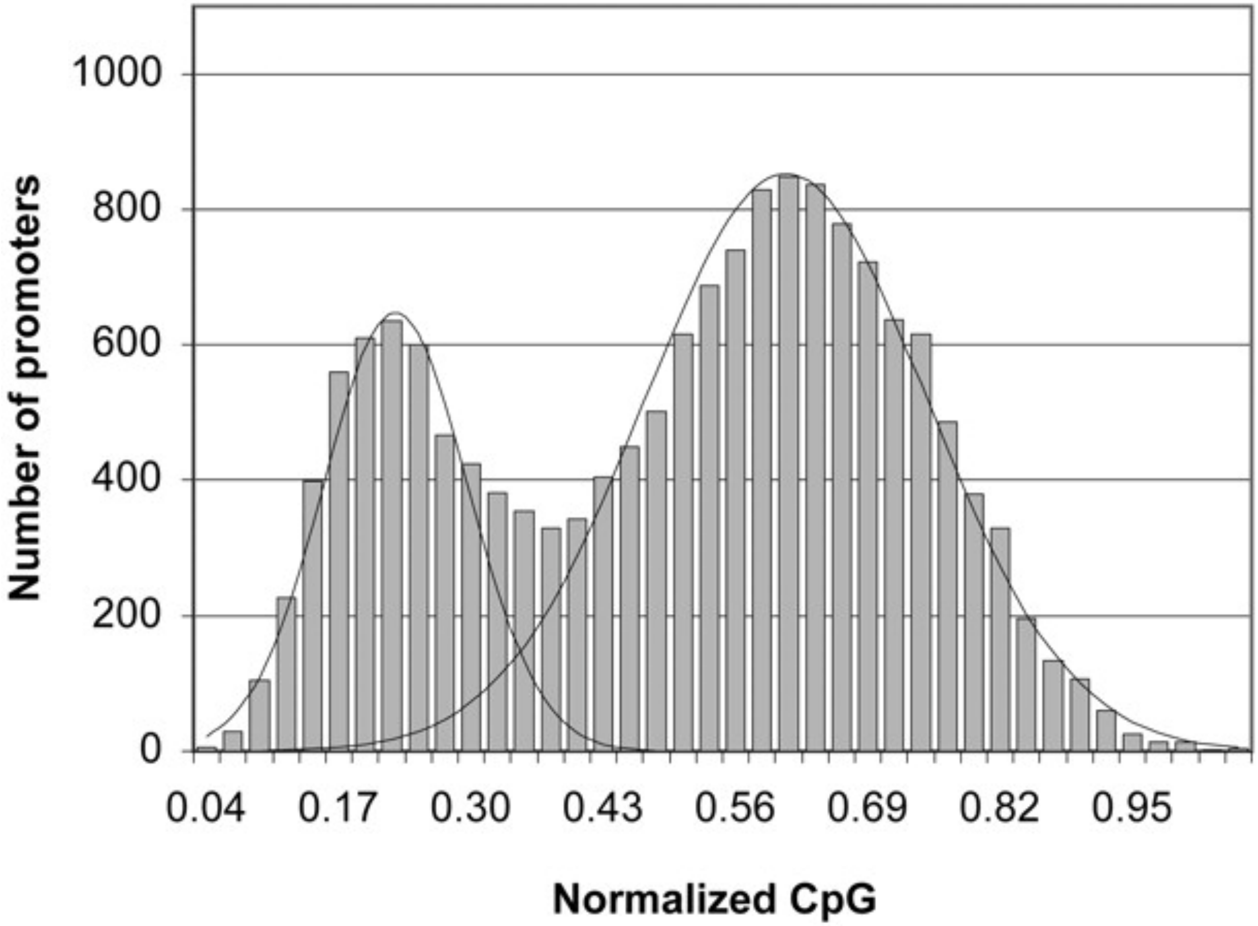


male and female genetics students, University of Connecticut in 1996

http://mindprod.com/jgloss/histogram.html

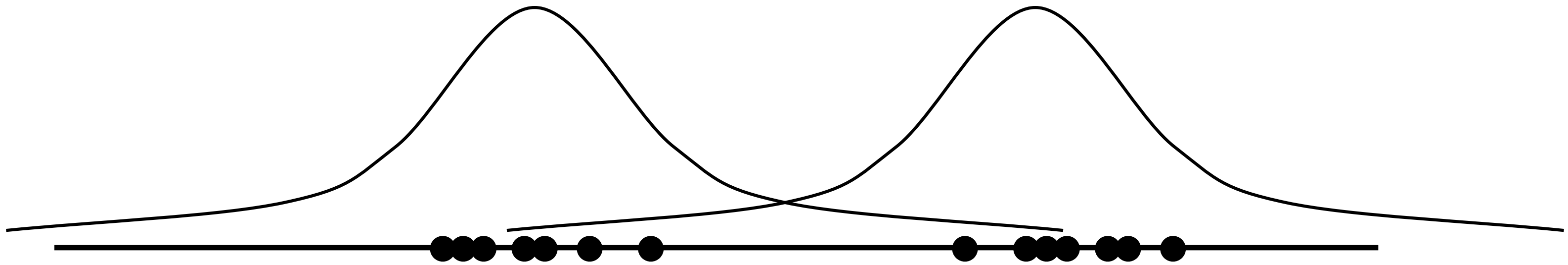
Another Real Example:

CpG content of human gene promoters



"A genome-wide analysis of CpG dinucleotides in the human genome distinguishes two distinct classes of promoters" Saxonov, Berg, and Brutlag, PNAS 2006;103:1412-1417

Gaussian Mixture Models / Model-based Clustering



Parameters θ

means	μ_1	μ_2
variances	σ_1^2	σ_2^2
mixing parameters	τ_1	$\tau_2 = 1 - \tau_1$

P.D.F. $\xrightarrow{\text{separately}}$ $f(x|\mu_1, \sigma_1^2) \quad f(x|\mu_2, \sigma_2^2)$

together

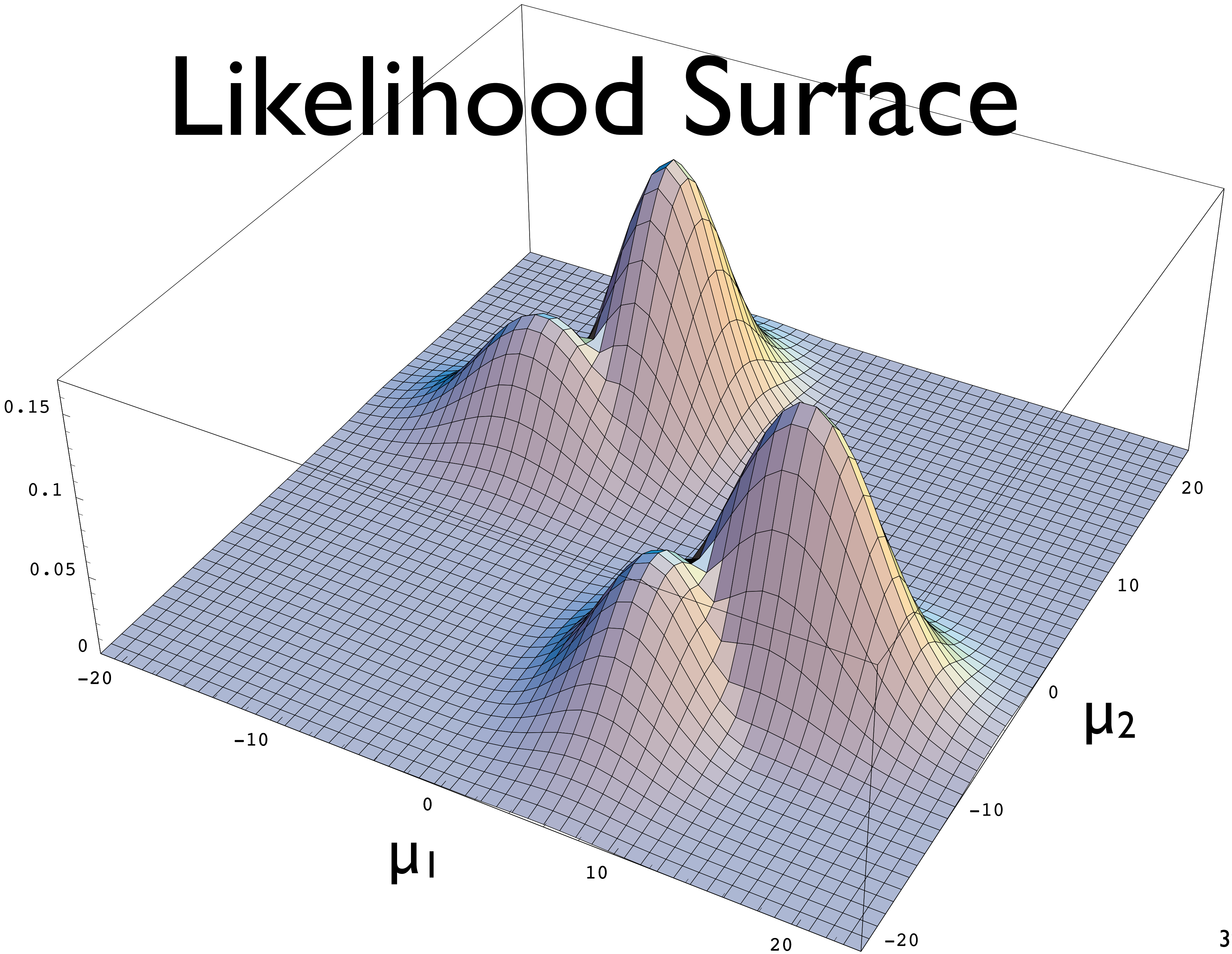
Likelihood $\boxed{\tau_1 f(x|\mu_1, \sigma_1^2) + \tau_2 f(x|\mu_2, \sigma_2^2)}$

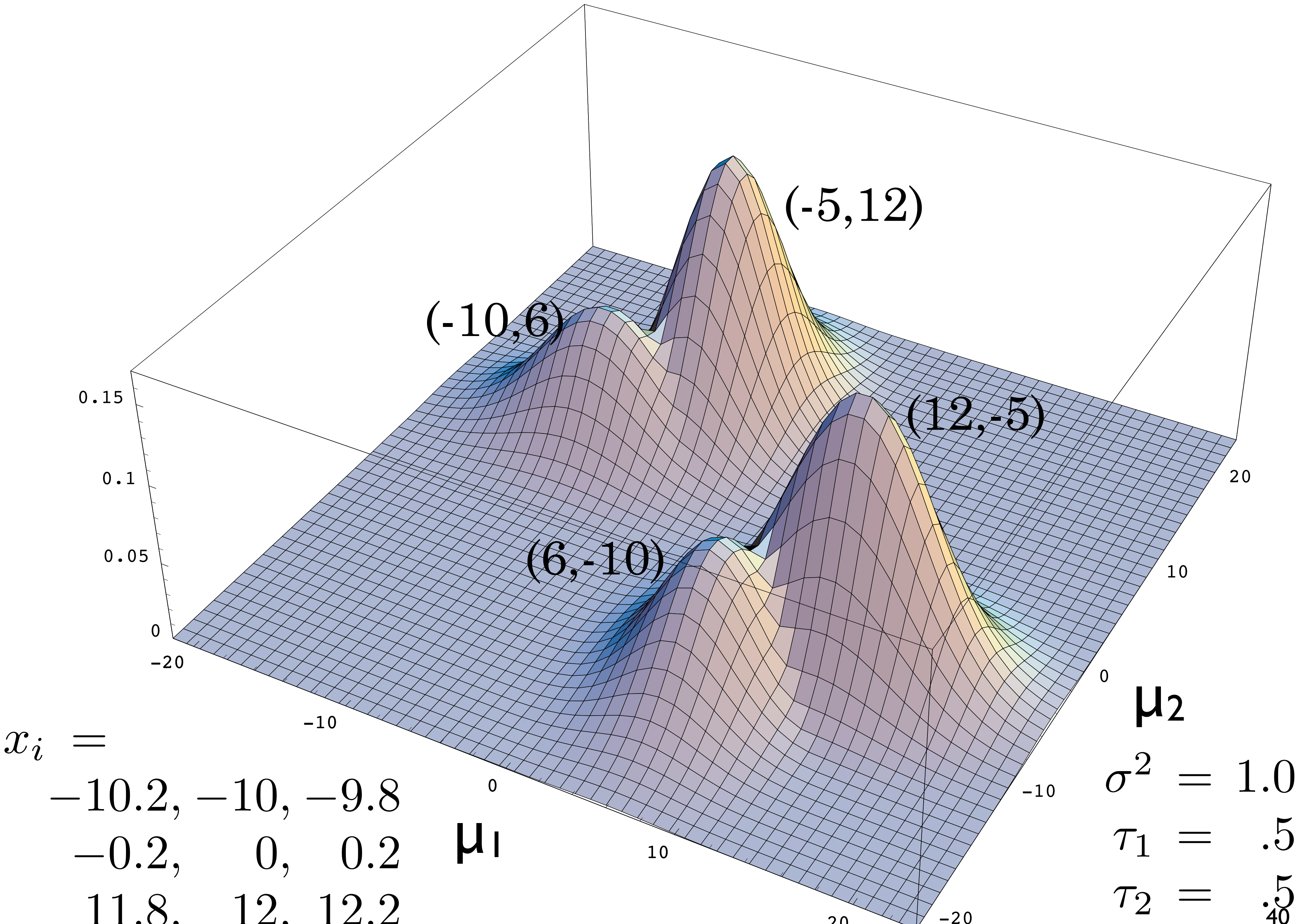
$$L(x_1, x_2, \ldots, x_n | \mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \tau_1, \tau_2)$$

$$= \prod_{i=1}^{n} \sum_{j=1}^{2} \tau_j f(x_i | \mu_j, \sigma_j^2)$$

No closed-form max

Likelihood Surface





(-5,12)
(-10,6)
(12,-5)
(6,-10)
0.15
0.1
0.05
0
-20
-10
0
10
20
μ1
μ2
x_i =
−10.2, −10, −9.8
−0.2, 0, 0.2
11.8, 12, 12.2
$\sigma^2 = 1.0$
$\tau_1 = .5$
$\tau_2 = .5$

A What-If Puzzle

Likelihood

$$L(x_1, x_2, \ldots, x_n | \overbrace{\mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \tau_1, \tau_2}^{\theta})$$

$$= \prod_{i=1}^{n} \sum_{j=1}^{2} \tau_j f(x_i | \mu_j, \sigma_j^2)$$

Messy: no closed form solution known for finding θ maximizing L

But *what if* we knew the *hidden data*?

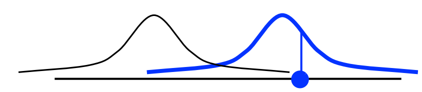
$$z_{ij} = \begin{cases} 1 & \text{if } x_i \text{ drawn from } f_j \\ 0 & \text{otherwise} \end{cases}$$

EM as Egg vs Chicken

Hat Trick 1

IF parameters θ known, could estimate z_{ij}

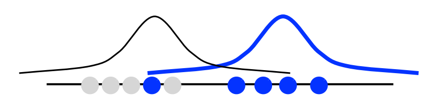
E.g., $|x_i - \mu_1|/\sigma_1 \gg |x_i - \mu_2|/\sigma_2 \Rightarrow P[z_{i1}=1] \ll P[z_{i2}=1]$



Hat Trick 2

IF z_{ij} known, could estimate parameters θ

E.g., only points in cluster 2 influence μ_2, σ_2



But we know neither; (optimistically) iterate:

Hat Trick 1

E-step: calculate expected z_{ij}, given parameters

Hat Trick 2

M-step: calculate "MLE" of parameters, given $E(z_{ij})$

Overall, a clever "hill-climbing" strategy

Simple Version: "Classification EM"

Not what's needed for homework, but may help clarify concepts

If $E[z_{ij}] < .5$, pretend $z_{ij} = 0$; $E[z_{ij}] > .5$, pretend it's 1

I.e., *classify* points as component 1 or 2

Now recalc θ, assuming that partition (standard MLE)

Then recalc $E[z_{ij}]$, assuming that θ

Then re-recalc θ, assuming new $E[z_{ij}]$, etc., etc.

"K-means clustering," essentially

"Full EM" is slightly more involved, (to account for uncertainty in classification) but this is the crux.

Full EM

x_i's are known; θ unknown. Goal is to find MLE θ of:

$$L(x_1, \ldots, x_n \mid \theta) \qquad \text{(hidden data likelihood)}$$

Would be easy *if* z_{ij}'s were known, i.e., consider:

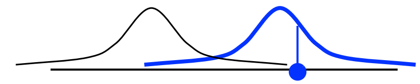
$$L(x_1, \ldots, x_n, z_{11}, z_{12}, \ldots, z_{n2} \mid \theta) \qquad \text{(complete data likelihood)}$$

But z_{ij}'s aren't known.

Instead, maximize *expected* likelihood of visible data

$$E(L(x_1, \ldots, x_n, z_{11}, z_{12}, \ldots, z_{n2} \mid \theta)),$$

where expectation is over distribution of hidden data (z_{ij}'s)



The E-step:

Find $E(z_{ij})$, i.e., $P(z_{ij}=1)$

Assume θ known & fixed

A (B): the event that x_i was drawn from f_1 (f_2)

D: the observed datum x_i

Expected value of z_{i1} is P(A|D) $E = 0 \cdot P(0) + 1 \cdot P(1)$

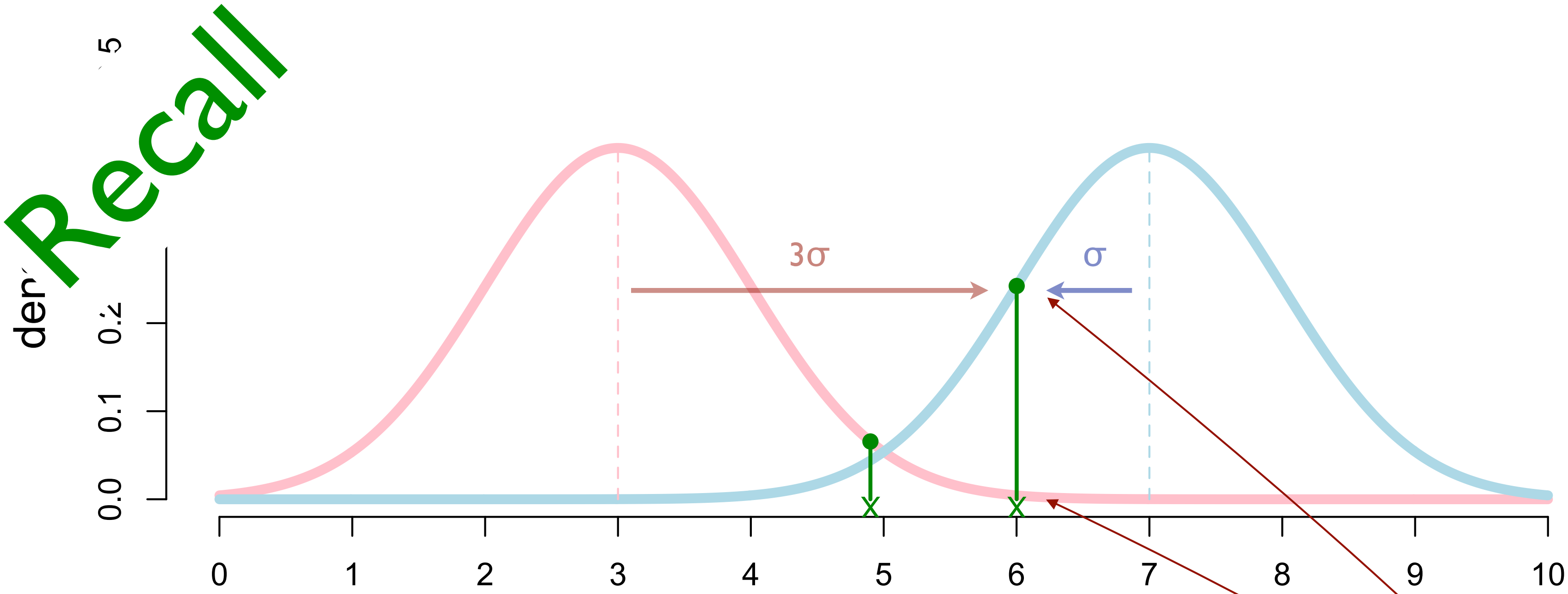
$$\boxed{P(A|D) = \frac{P(D|A)P(A)}{P(D)}}$$

$$\begin{aligned} P(D) &= P(D|A)P(A) + P(D|B)P(B) \\ &= f_1(x_i|\theta_1)\,\tau_1 + f_2(x_i|\theta_2)\,\tau_2 \end{aligned}$$

Repeat for each x_i

Note: denominator = sum of numerators – i.e. that which normalizes sum to 1 (typical Bayes)

A Hat Trick



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$$P(\mu = 7 | X \approx 6) = \frac{P(X \approx 6 | \mu = 7) P(\mu = 7)}{P(X \approx 6)}$$

$$= \frac{0.5 P(X \approx 6 | \mu = 7)}{0.5 P(X \approx 6 | \mu = 3) + 0.5 P(X \approx 6 | \mu = 7)}$$

$$\approx \frac{f(X = 6 | \mu = 7)\delta}{f(X = 6 | \mu = 3)\delta + f(X = 6) | \mu = 7)\delta}, \text{ so}$$

$$P(\mu = 7 | X = 6) = \frac{f(X = 6 | \mu = 7)}{f(X = 6 | \mu = 3) + f(X = 6) | \mu = 7)} \approx 0.982$$

f = normal density

Complete Data Likelihood

Recall:

$$z_{1j} \;=\; \begin{cases} 1 & \text{if } x_1 \text{ drawn from } f_j \\ 0 & \text{otherwise} \end{cases}$$

so, correspondingly,

$$L(x_1, z_{1j} \mid \theta) \;=\; \begin{cases} \tau_1 f_1(x_1 \mid \theta) & \text{if } z_{11} = 1 \\ \tau_2 f_2(x_1 \mid \theta) & \text{otherwise} \end{cases}$$

equal, if z_{ij} are 0/1

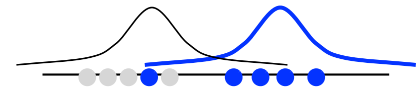
Formulas with "if's" are messy; can we blend more smoothly?
Yes, many possibilities. Idea 1:

$$L(x_1, z_{1j} \mid \theta) \;=\; z_{11} \cdot \tau_1 f_1(x_1 \mid \theta) + z_{12} \cdot \tau_2 f_2(x_1 \mid \theta)$$

Idea 2 (Better):

$$L(x_1, z_{1j} \mid \theta) \;=\; (\tau_1 f_1(x_1 \mid \theta))^{z_{11}} \cdot (\tau_2 f_2(x_1 \mid \theta))^{z_{12}}$$

M-step:



Find θ maximizing E(log(Likelihood))

(For simplicity, assume $\sigma_1 = \sigma_2 = \sigma; \tau_1 = \tau_2 = \tau = 0.5$)

$$L(\vec{x}, \vec{z} \mid \theta) = \prod_{i=1}^{n} \frac{\tau}{\sqrt{2\pi\sigma^2}} \exp\left(-\sum_{j=1}^{2} z_{ij} \frac{(x_i - \mu_j)^2}{2\sigma^2} \right)$$

$$E[\log L(\vec{x}, \vec{z} \mid \theta)] = E\left[\sum_{i=1}^{n} \left(\log \tau - \frac{1}{2} \log(2\pi\sigma^2) - \sum_{j=1}^{2} z_{ij} \frac{(x_i - \mu_j)^2}{2\sigma^2} \right) \right]$$

wrt dist of z_{ij}

$$= \sum_{i=1}^{n} \left(\log \tau - \frac{1}{2} \log(2\pi\sigma^2) - \sum_{j=1}^{2} E[z_{ij}] \frac{(x_i - \mu_j)^2}{2\sigma^2} \right)$$

Find θ maximizing this as before, using $E[z_{ij}]$ found in E-step. Result:

$\boxed{\mu_j = \sum_{i=1}^{n} E[z_{ij}] x_i / \sum_{i=1}^{n} E[z_{ij}]}$ (intuit: avg, weighted by subpop prob)

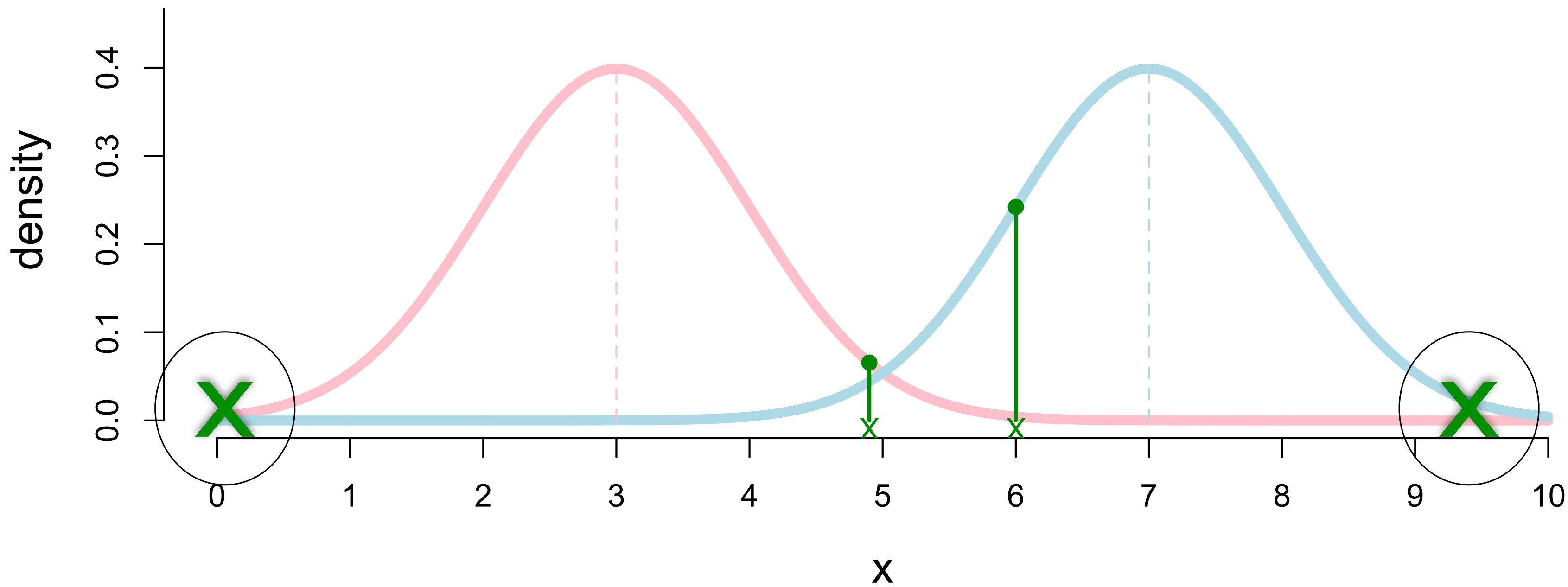
Recall

Hat Trick 2 (cont.)

Note 2: red/blue separation is just like the M-step of EM *if values of the hidden variables (z_{ij}) were known.*

What if they're not? E.g., what would you do if some of the slips you pulled had coffee spilled on them, obscuring color?

> If they were half way between means of the others?
> If they were on opposite sides of the means of the others



M-step:calculating mu's

$$\boxed{\mu_j = \sum_{i=1}^{n} E[z_{ij}]x_i / \sum_{i=1}^{n} E[z_{ij}]}$$

In words: μ_j is the average of the observed x_i's, weighted by the probability that x_i was sampled from component j.

old E's

							row sum	avg
$E[z_{i1}]$	0.99	0.98	0.7	0.2	0.03	0.01	2.91	
$E[z_{i2}]$	0.01	0.02	0.3	0.8	0.97	0.99	3.09	
x_i	9	10	11	19	20	21	90	15
$E[z_{i1}]x_i$	8.9	9.8	7.7	3.8	0.6	0.2	31.0	10.66
$E[z_{i1}]x_i$	0.1	0.2	3.3	15.2	19.4	20.8	59.0	19.09

new μ's

2 Component Mixture

$$\sigma_1 = \sigma_2 = 1; \;\; \tau = 0.5$$

			mu1	-20.00		-6.00		-5.00		-4.99
			mu2	6.00		0.00		3.75		3.75
x1	**-6**		**z11**		5.11E-12		1.00E+00		1.00E+00	
x2	**-5**		**z21**		2.61E-23		1.00E+00		1.00E+00	
x3	**-4**		**z31**		1.33E-34		9.98E-01		1.00E+00	
x4	**0**		**z41**		9.09E-80		1.52E-08		4.11E-03	
x5	**4**		**z51**		6.19E-125		5.75E-19		2.64E-18	
x6	**5**		**z61**		3.16E-136		1.43E-21		4.20E-22	
x7	**6**		**z71**		1.62E-147		3.53E-24		6.69E-26	

Essentially converged in 2 iterations

(Excel spreadsheet on course web)

EM Summary

Fundamentally a maximum likelihood parameter estimation problem; broader than just Gaussian

Useful if 0/1 hidden data, and if analysis would be more tractable if hidden data z were known

Iterate:

E-step: estimate E(z) for each z, given θ

M-step: estimate θ maximizing E[log likelihood] given E[z] [where "E[logL]" is wrt random z ~ E[z] = p(z=1)]

Bayes

MLE

EM Issues

Under mild assumptions, EM is guaranteed to increase likelihood with every E-M iteration, hence will *converge*.

But it may converge to a *local*, not global, max. (Recall the 4-bump surface...)

Issue is intrinsic (probably), since EM is often applied to problems (including clustering, above) that are *NP-hard* (so fast alg is unlikely)

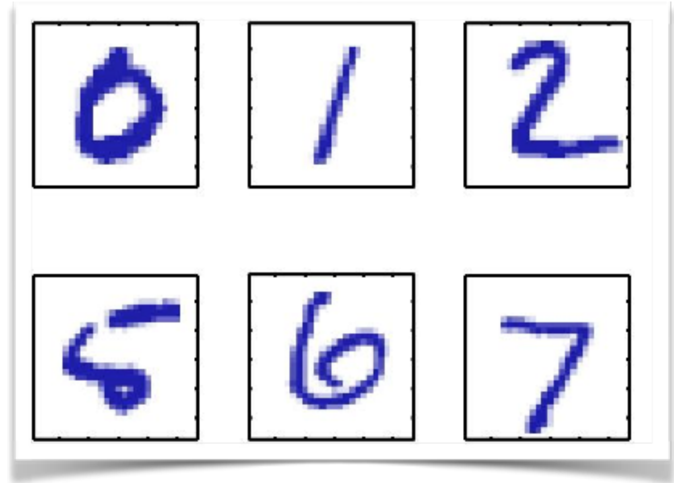
Nevertheless, widely used, often effective

Applications

- Clustering is a remarkably successful exploratory data analysis tool
  - Web-search, information retrieval, gene-expression, ...
  - Model-based approach above is one of the leading ways to do it
- Gaussian mixture models widely used
  - With many components, empirically match arbitrary distribution
  - Often well-justified, due to "hidden parameters" driving the visible data
- EM is extremely widely used for "hidden-data" problems
  - Hidden Markov Models – speech recognition, DNA analysis, ...

A "Machine Learning" Example

Handwritten Digit Recognition



Given: 10^4 unlabeled, scanned images of handwritten digits, say 25 x 25 pixels,

Goal: automatically classify new examples

Possible Method:

Each image is a point in $\mathbb{R}^{625}$; the "ideal" 7, say, is one such point; model other 7's as a Gaussian cloud around it

Do EM, as above, but 10 components in 625 dimensions instead of 2 components in 1 dimension

"Recognize" a new digit by best fit to those 10 models, i.e., basically max E-step probability

Machine Learning / Data Analytics Hot Topics Now. Why?

Advances in theoretical foundations

Including probabilistic and statistical modeling

Advances in algorithms

Advances in computational power

Floods of data

Floods of applications

Science, engineering, medicine, security, commerce, …