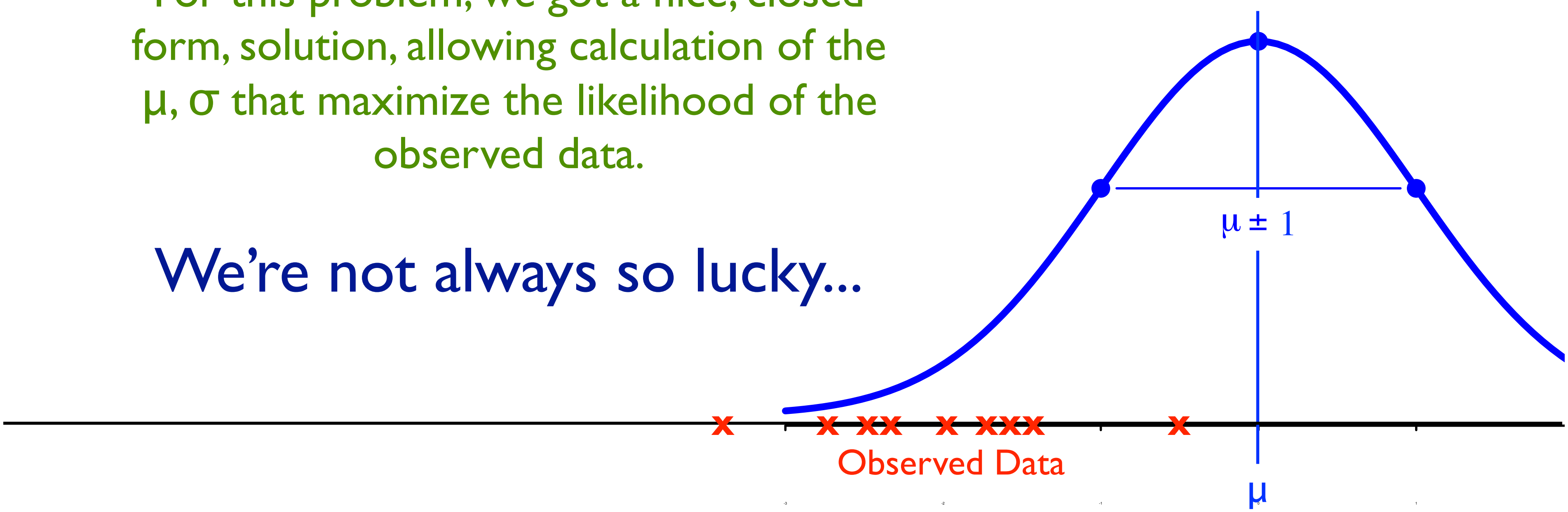
EM

The Expectation-Maximization Algorithm

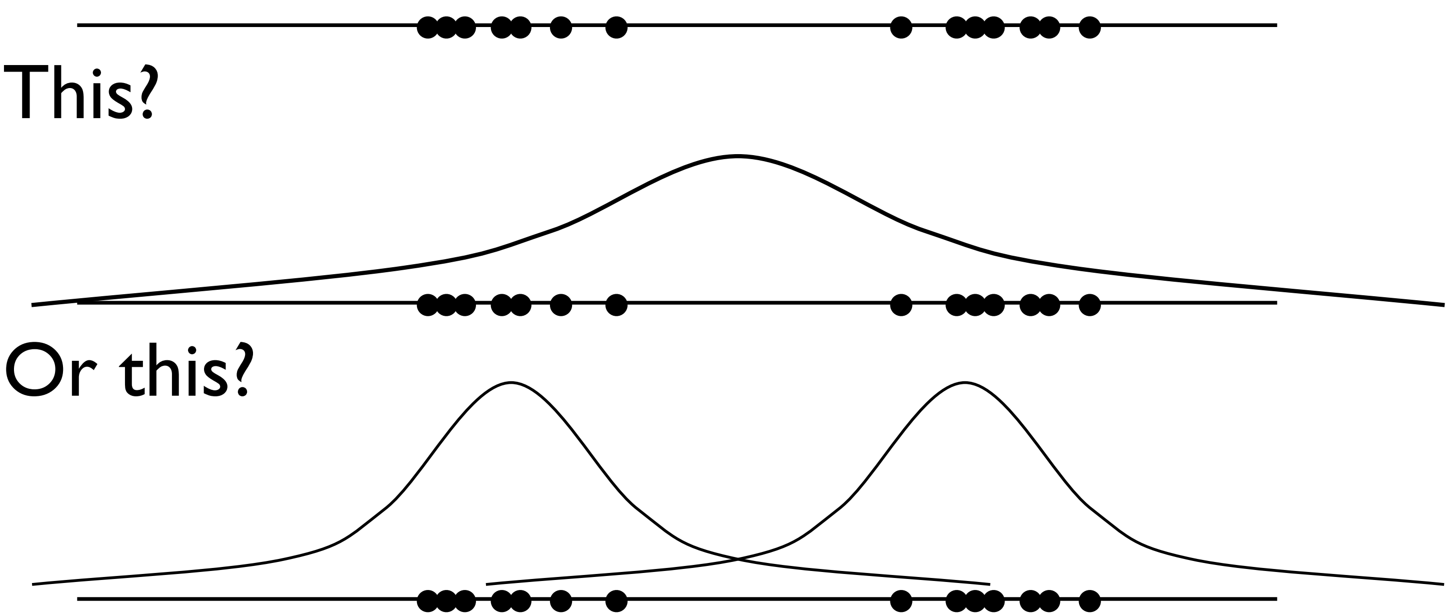
Last lecture:
How to estimate μ given data

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...



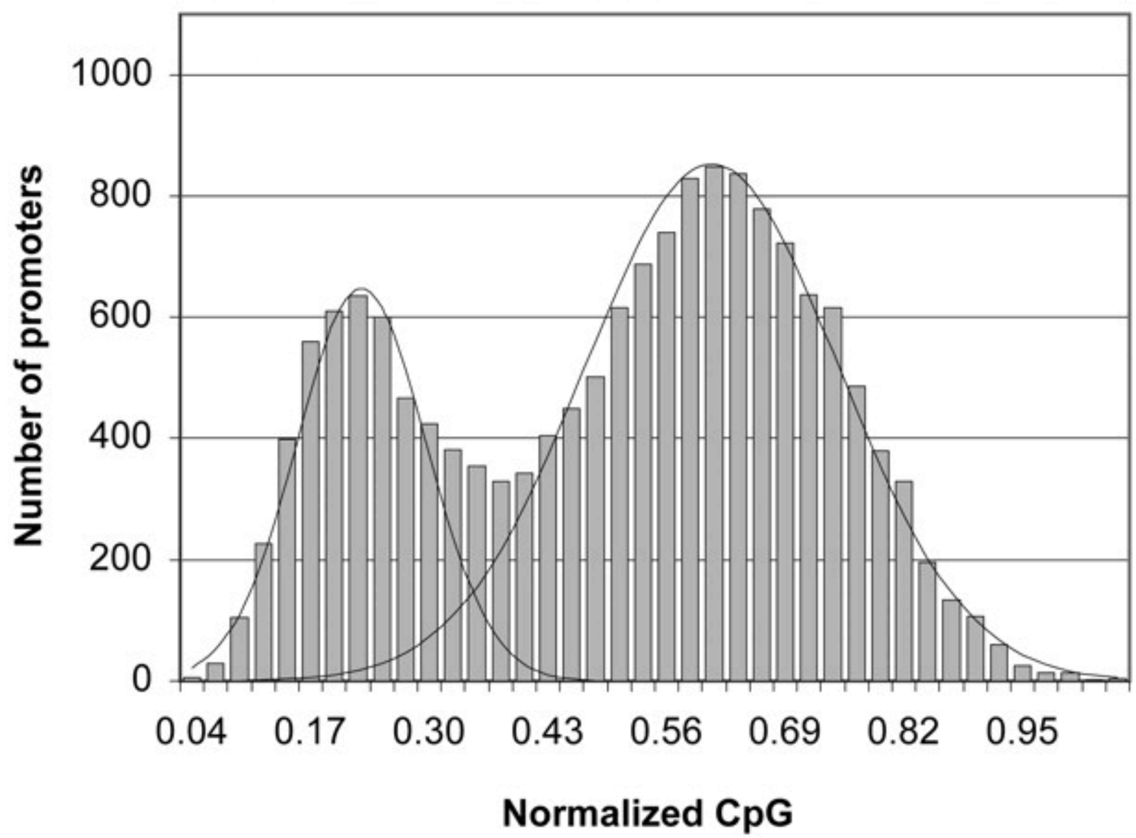
More Complex Example



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

A 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

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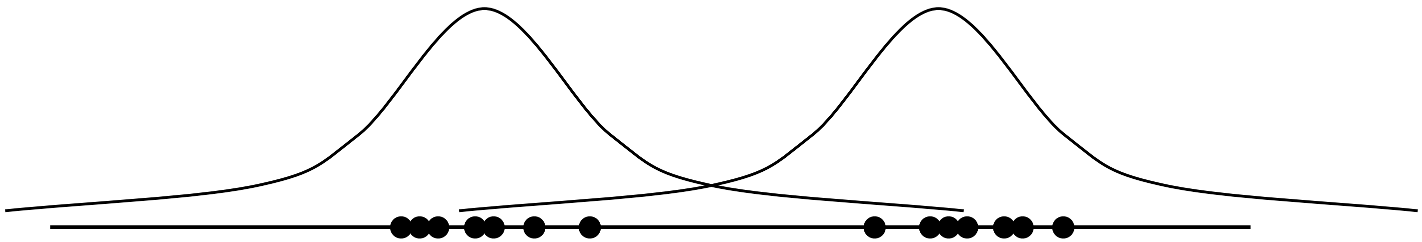
Gaussian Mixture Models / Model-based Clustering



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. $\quad f(x|\mu_1, \sigma_1^2) \quad f(x|\mu_2, \sigma_2^2)$

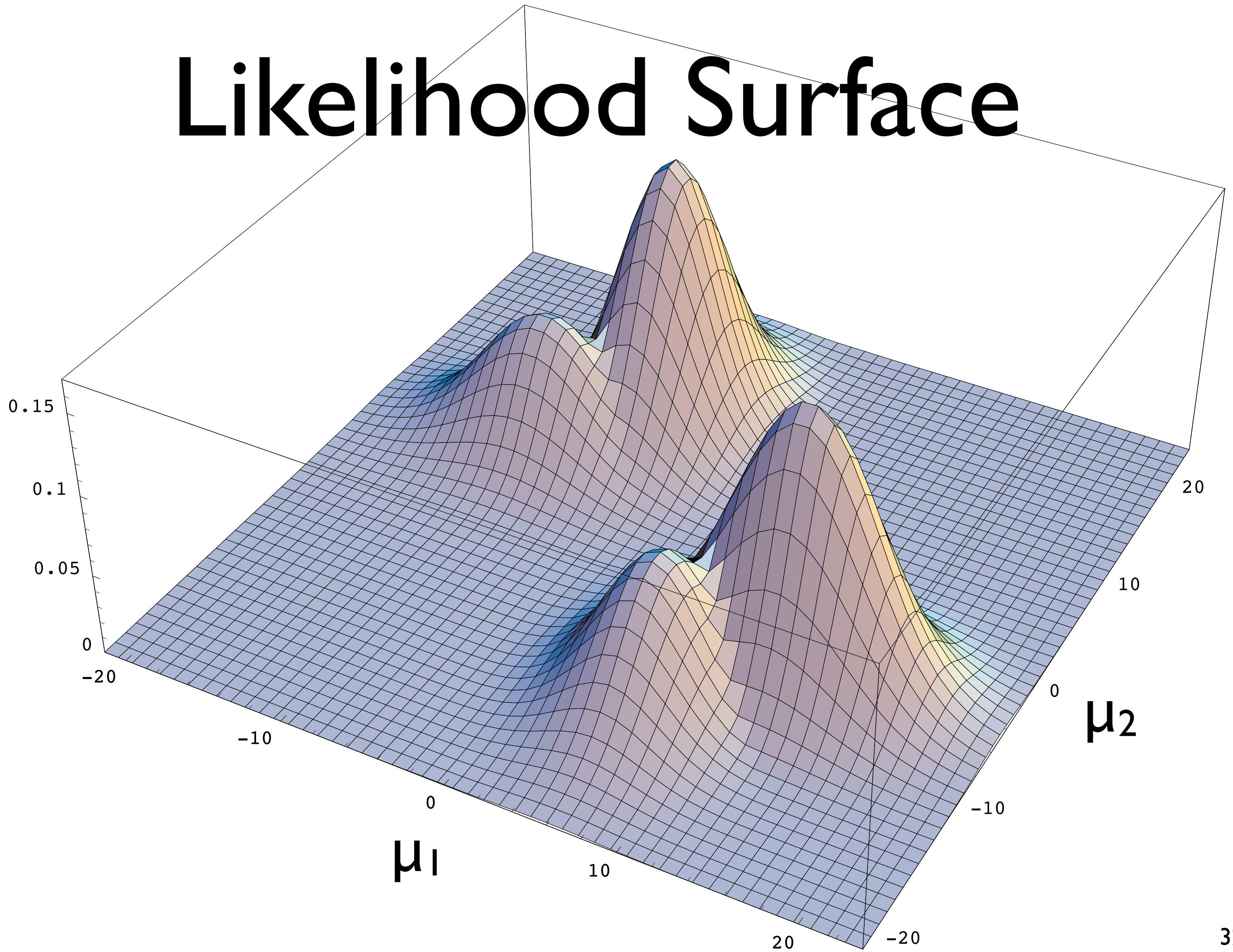
Likelihood

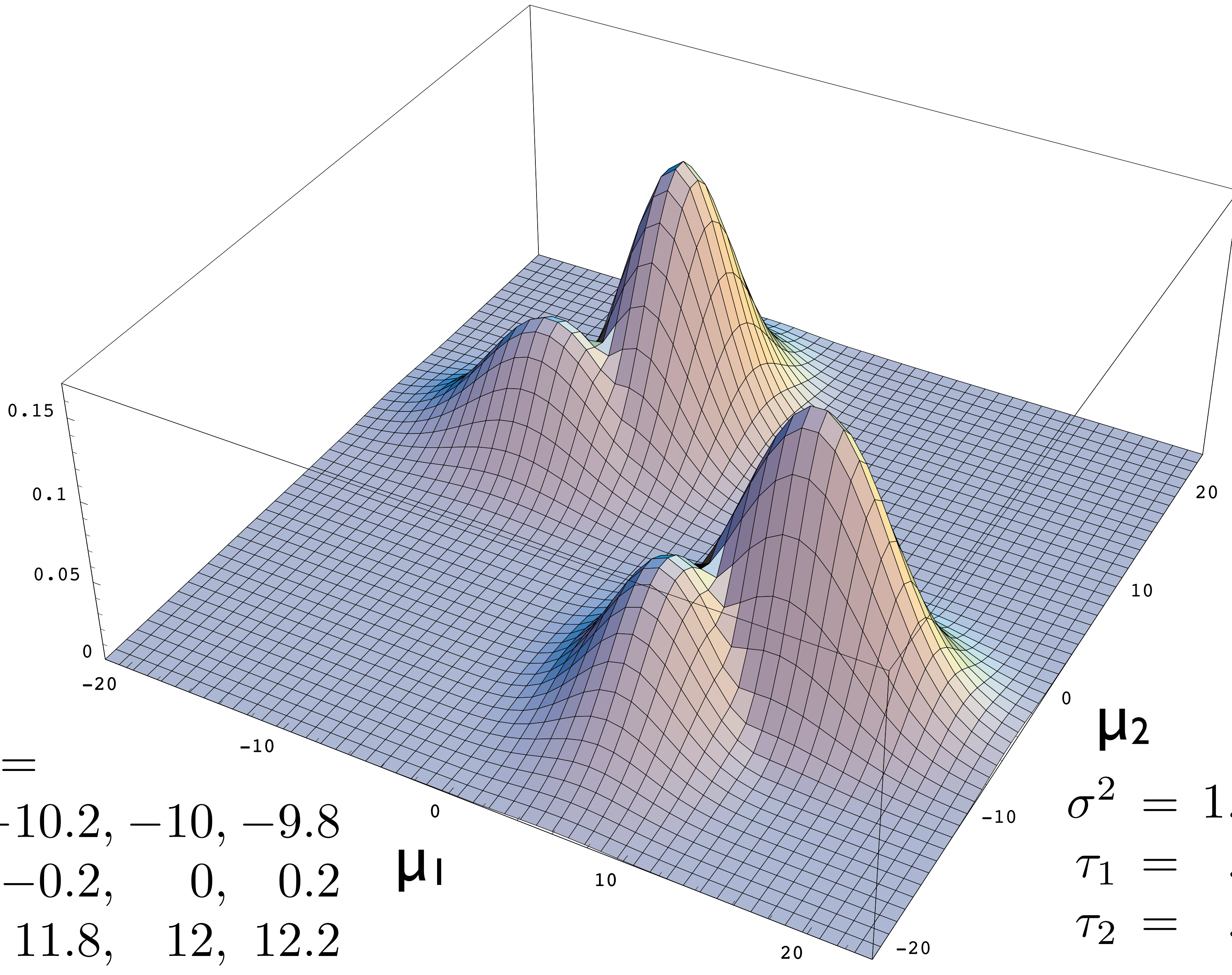
$$L(x_1, x_2, \ldots, x_n | \mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \tau_1, \tau_2)$$

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

No closed-form max

Likelihood Surface





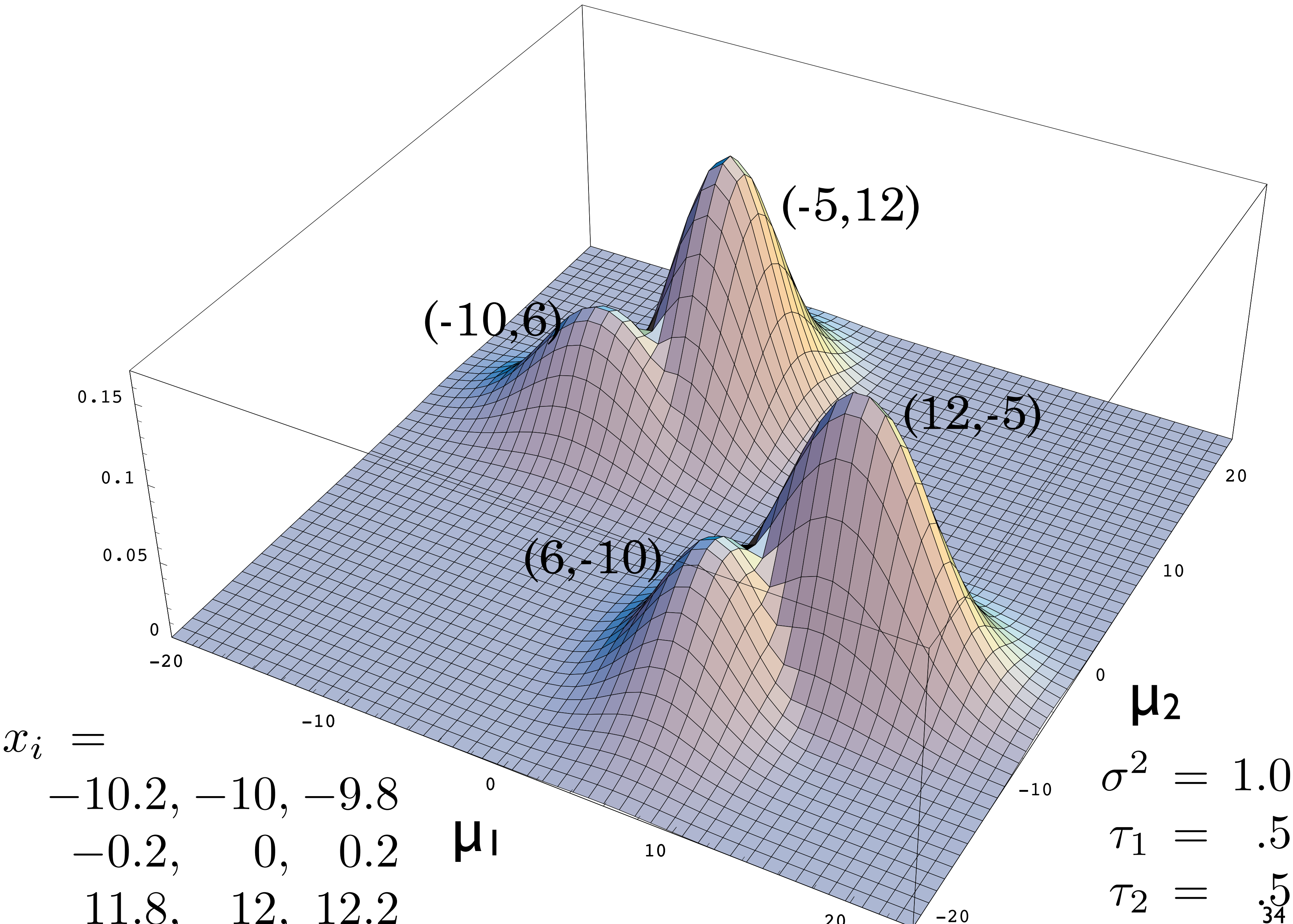
$x_i =$

$$\begin{array}{rrr} -10.2, & -10, & -9.8 \\ -0.2, & 0, & 0.2 \\ 11.8, & 12, & 12.2 \end{array}$$

$\sigma^2 = 1.0$

$\tau_1 = .5$

$\tau_2 = .5$


(-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

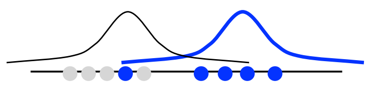
But *what if* we knew the *hidden data*?

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

EM as Egg vs Chicken

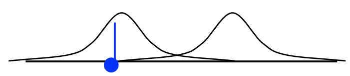
IF z_{ij} known, could estimate parameters θ

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



IF parameters θ known, could estimate z_{ij}

E.g., if $|x_i - \mu_1|/\sigma_1 << |x_i - \mu_2|/\sigma_2$, then $z_{i1} >> z_{i2}$



But we know neither; (optimistically) iterate:

E: calculate expected z_{ij}, given parameters

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

Overall, a clever "hill-climbing" strategy

Simple Version: "Classification EM"

If z_{ij} < .5, pretend it's 0; z_{ij} > .5, pretend it's 1

I.e., *classify* points as component 0 or 1

Now recalc θ, assuming that partition

Then recalc z_{ij} , assuming that θ

Then re-recalc θ, assuming new z_{ij}, etc., etc.

"Full EM" is a bit more involved, but this is the crux.

Full EM

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

$$L(x_1, \ldots, x_n \mid \theta)$$ (hidden data likelihood)

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

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

$E = 0 \cdot P(0) + 1 \cdot P(1)$

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

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

Repeat for each x_i

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,

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

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 $\sigma_1 = \sigma_2 = \sigma; \tau_1 = \tau_2 = .5 = \tau$)

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

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

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

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)

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)

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

EM Summary

Fundamentally a maximum likelihood parameter estimation problem

Useful if hidden data, and if analysis is more tractable when 0/1 hidden data z 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)]

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* (next 3 weeks!)

Nevertheless, widely used, often effective