CSE 427

Autumn 2015

MLE, EM

MyoD

http://www.rcsb.org/pdb/explore/jmol.do?structureId=1MDY&bionumber=1

Outline

MLE: Maximum Likelihood Estimators

EM: the Expectation Maximization Algorithm

Learning From Data: MLE

Maximum Likelihood Estimators

Parameter Estimation

Given: independent samples $x_1, x_2, \ldots, x_n$ from a parametric distribution $f(x|\theta)$

Goal: estimate θ.

E.g.: Given sample HHTTTTTHTHTTTHH of (possibly biased) coin flips, estimate

$$\theta = \text{probability of Heads}$$

$f(x|\theta)$ is the Bernoulli probability mass function with parameter θ

Likelihood

$P(x \mid \theta)$: Probability of event x given *model* θ

Viewed as a function of x (fixed θ), it's a *probability*

E.g., $\Sigma_x P(x \mid \theta) = 1$

Viewed as a function of θ (fixed x), it's called *likelihood*

E.g., $\Sigma_\theta P(x \mid \theta)$ can be anything; *relative* values of interest.

E.g., if θ = prob of heads in a sequence of coin flips then
$P(HHTHH \mid .6) > P(HHTHH \mid .5)$,

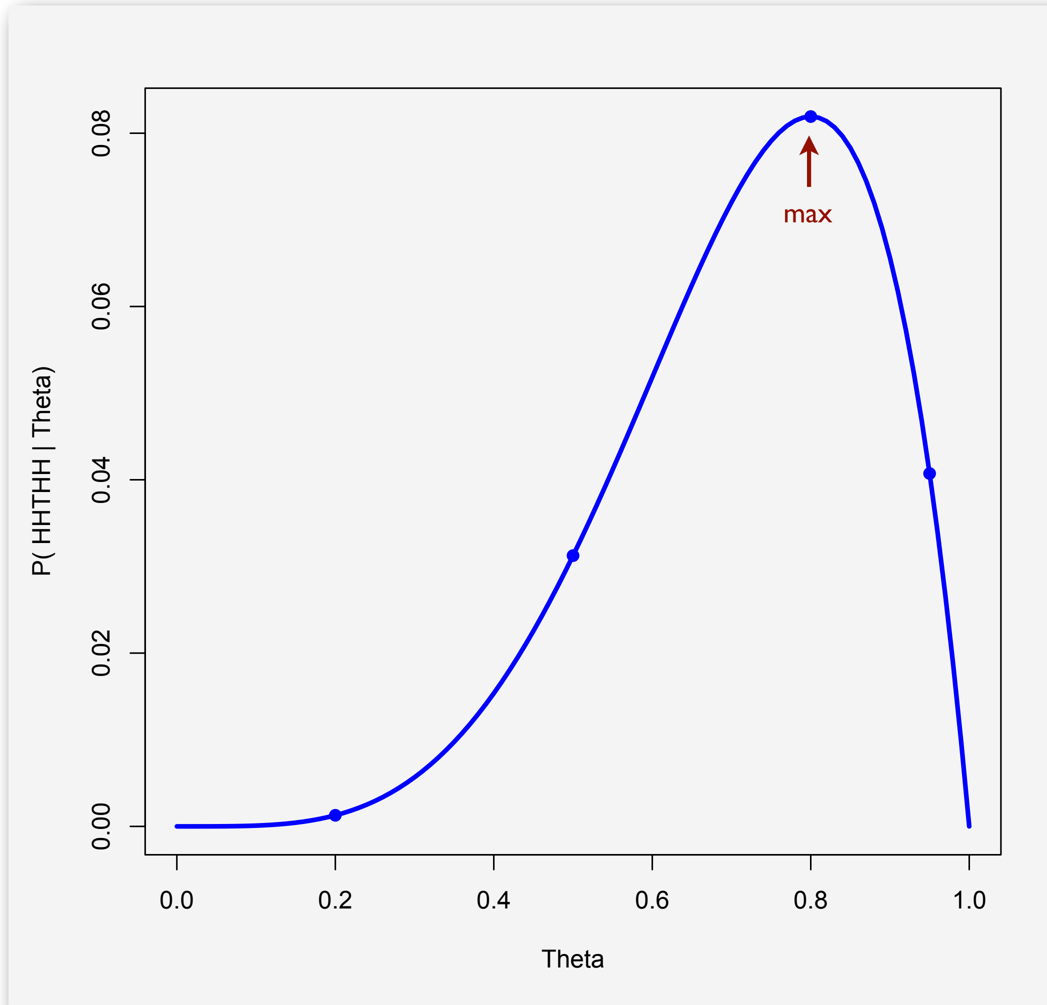
I.e., event HHTHH is *more likely* when $\theta = .6$ than $\theta = .5$

And what θ make HHTHH *most* likely?

Likelihood Function

P(HHTHH | θ):
Probability of HHTHH,
given P(H) = θ:

θ	$\theta^4(1-\theta)$
0.2	0.0013
0.5	0.0313
0.8	0.0819
0.95	0.0407



Maximum Likelihood Parameter Estimation

One (of many) approaches to param. est.

Likelihood of (indp) observations $x_1, x_2, ..., x_n$

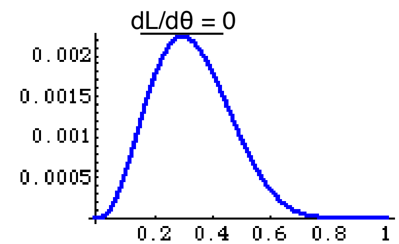
$$L(x_1, x_2, \ldots, x_n \mid \theta) = \prod_{i=1}^{n} f(x_i \mid \theta)$$

As a function of θ, what θ maximizes the likelihood of the data actually observed

Typical approach: $\frac{\partial}{\partial\theta} L(\vec{x} \mid \theta) = 0$ or $\frac{\partial}{\partial\theta} \log L(\vec{x} \mid \theta) = 0$

Example 1

n independent coin flips, $x_1, x_2, ..., x_n$; n_0 tails, n_1 heads, $n_0 + n_1 = n$; θ = probability of heads



$$
\begin{aligned}
L(x_1, x_2, \ldots, x_n \mid \theta) &= (1-\theta)^{n_0}\theta^{n_1} \\
\log L(x_1, x_2, \ldots, x_n \mid \theta) &= n_0 \log(1-\theta) + n_1 \log\theta \\
\frac{\partial}{\partial\theta} \log L(x_1, x_2, \ldots, x_n \mid \theta) &= \frac{-n_0}{1-\theta} + \frac{n_1}{\theta}
\end{aligned}
$$

Setting to zero and solving:

$$
\boxed{\hat{\theta} = \frac{n_1}{n}}
$$

Observed fraction of successes in *sample* is MLE of success probability in *population*

(Also verify it's max, not min, & not better on boundary)

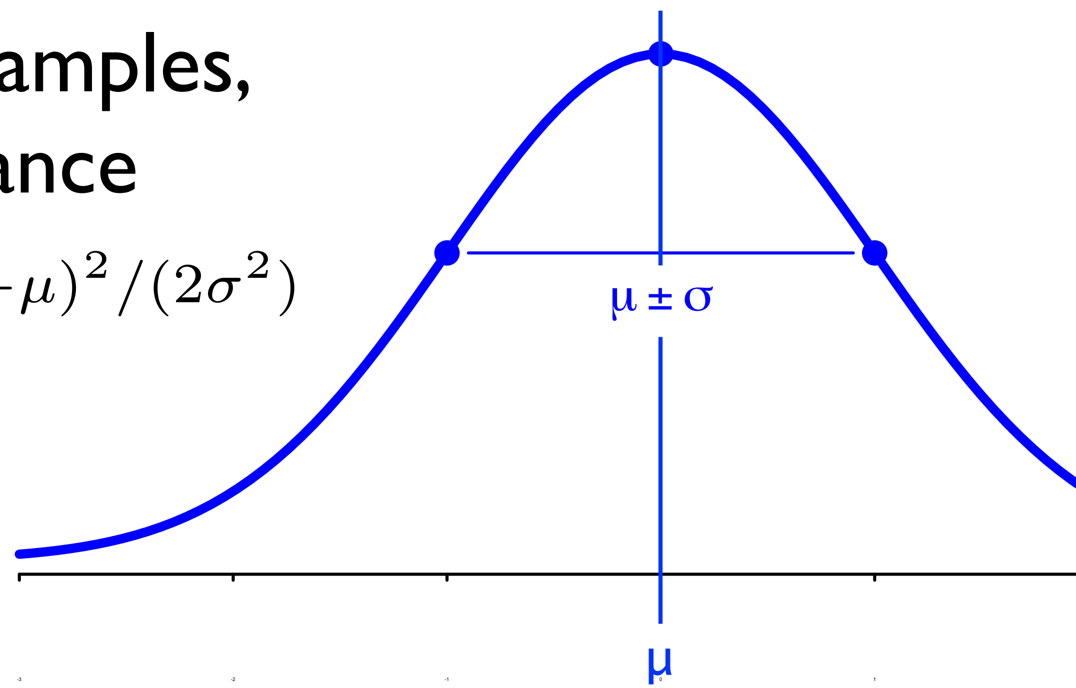
Parameter Estimation

Given: indp samples $x_1, x_2, ..., x_n$ from a parametric distribution $f(x|\theta)$, ***estimate:*** θ.

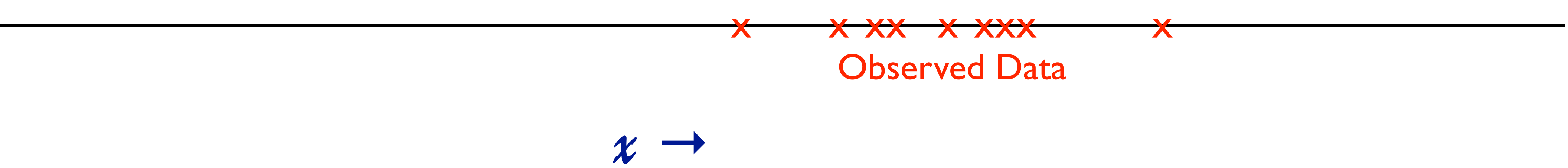
E.g.: Given *n normal* samples, estimate mean & variance

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/(2\sigma^2)}$$

$$\theta = (\mu, \sigma^2)$$

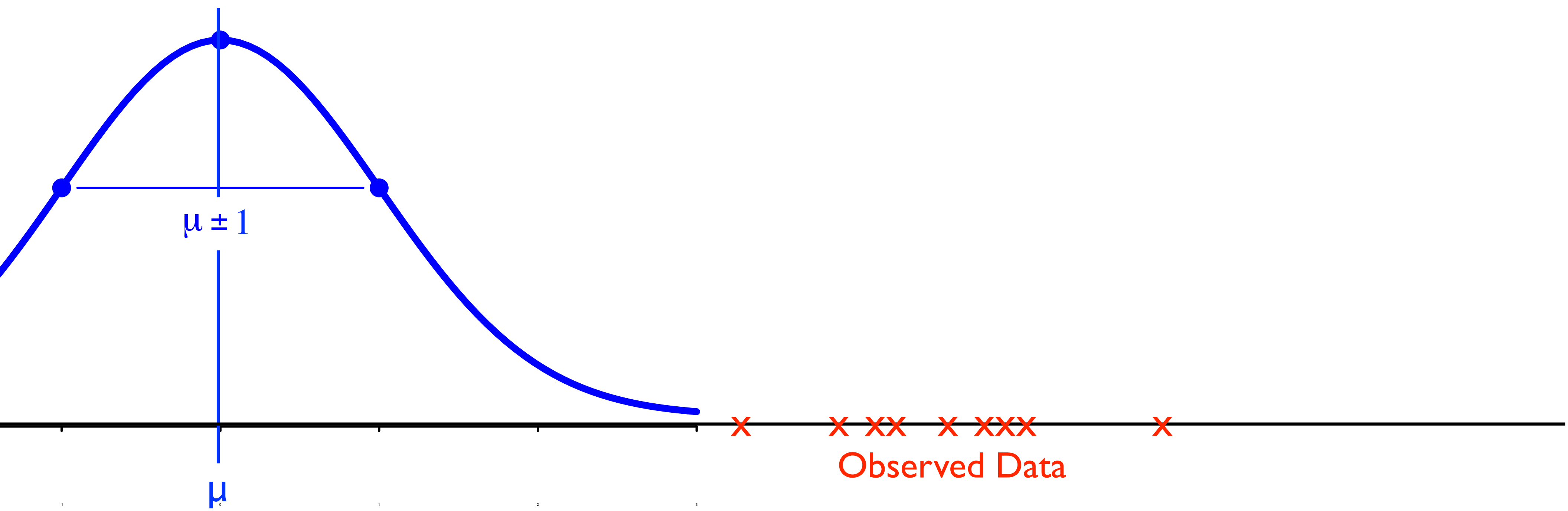


Ex2: I got data; a little birdie tells me it's normal, and promises $\sigma^2 = 1$



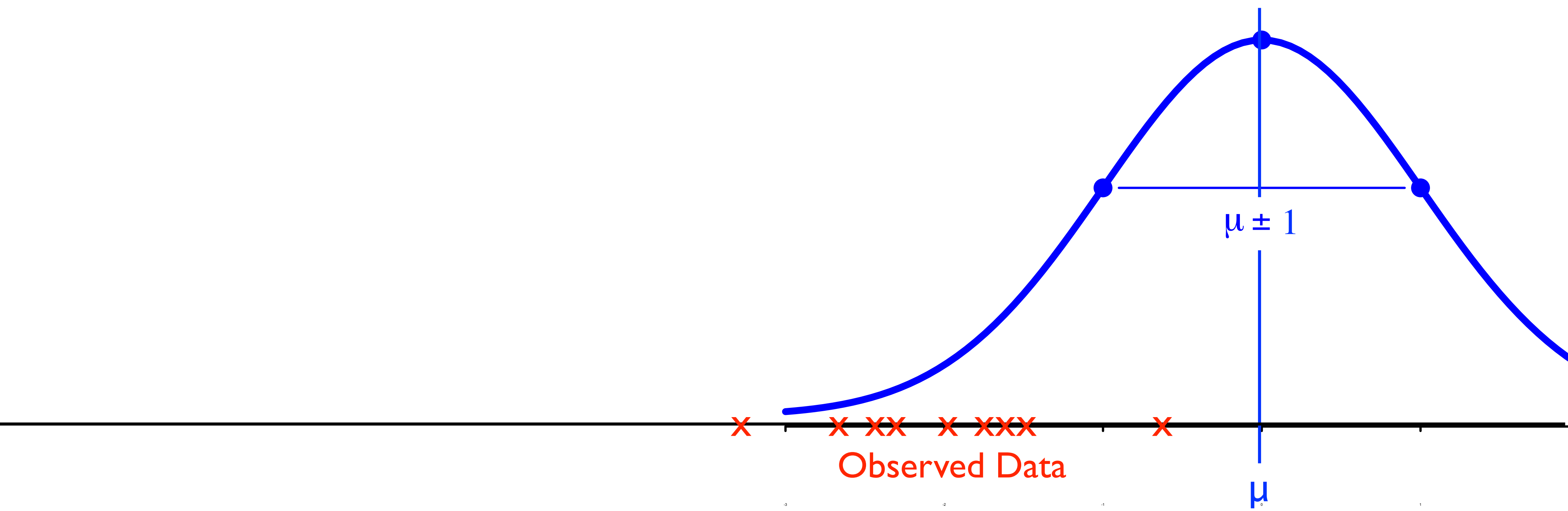
Which is more likely: (a) this?

μ unknown, $\sigma^2 = 1$



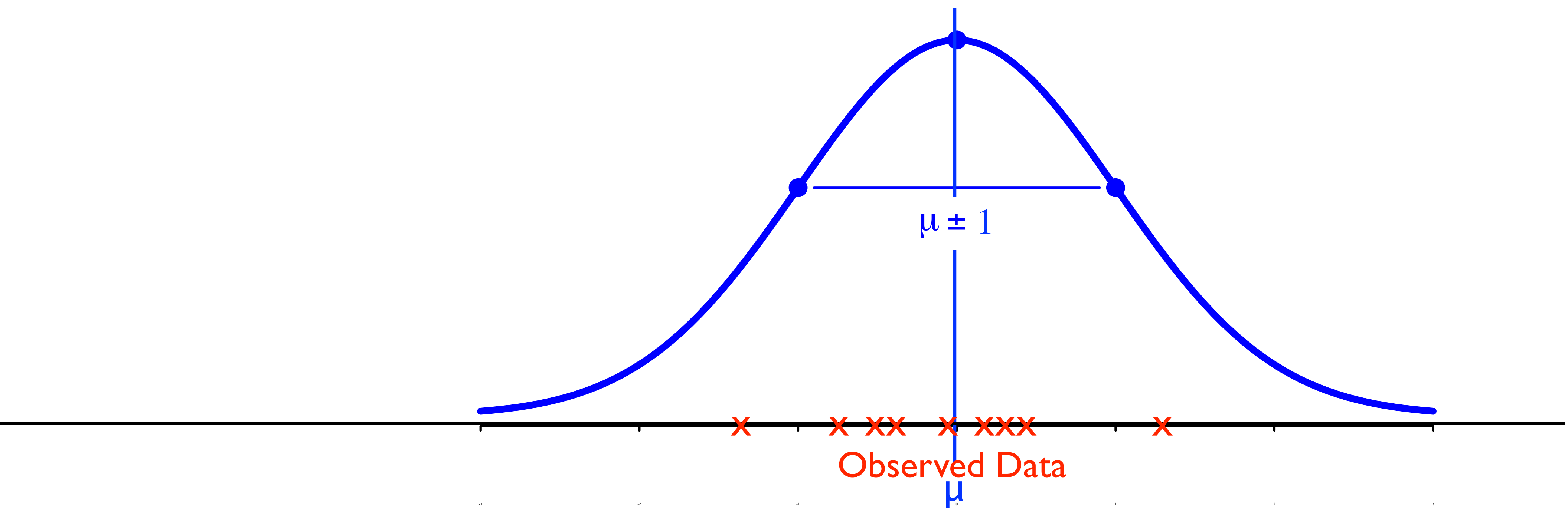
Which is more likely: (b) or this?

μ unknown, $\sigma^2 = 1$



Which is more likely: (c) or *this*?

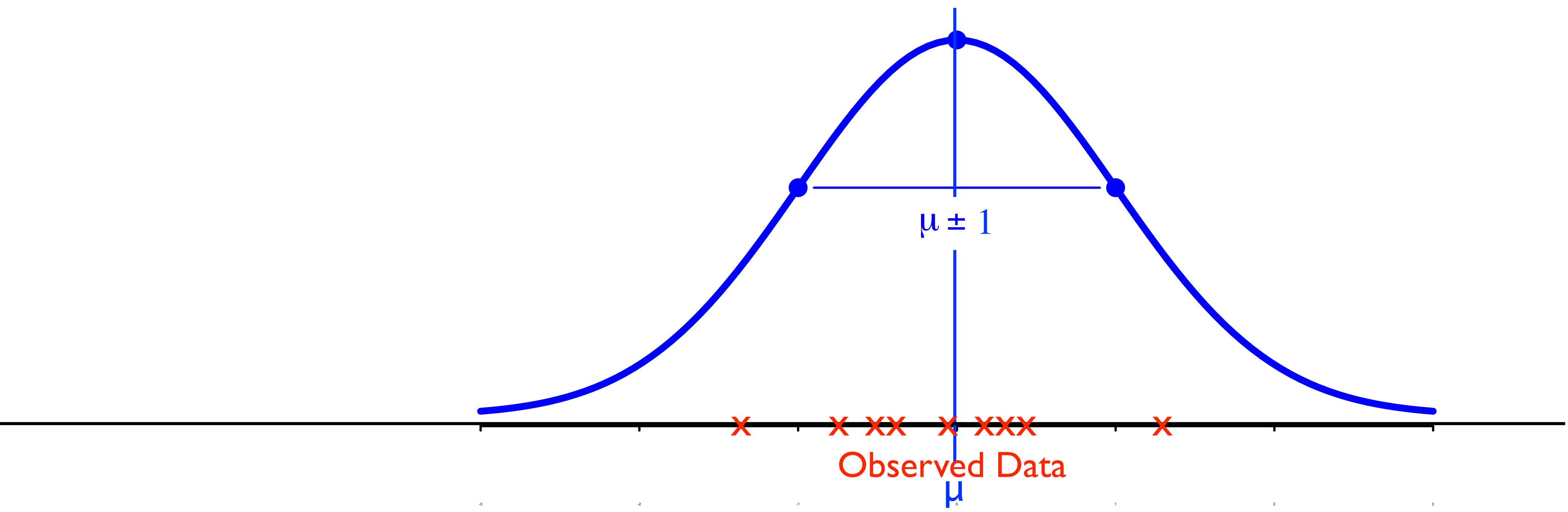
μ unknown, $\sigma^2 = 1$



Which is more likely: (c) or *this*?

μ unknown, $\sigma^2 = 1$

Looks good by eye, but how do I optimize my estimate of μ ?



Ex. 2: $x_i \sim N(\mu, \sigma^2),\ \sigma^2 = 1,\ \mu$ unknown

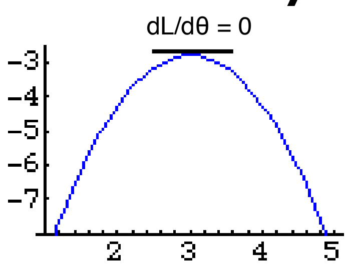
$$L(x_1, x_2, \ldots, x_n|\theta) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}} e^{-(x_i-\theta)^2/2}$$

$$\ln L(x_1, x_2, \ldots, x_n|\theta) = \sum_{i=1}^{n} -\frac{1}{2}\ln(2\pi) - \frac{(x_i-\theta)^2}{2}$$

$$\frac{d}{d\theta}\ln L(x_1, x_2, \ldots, x_n|\theta) = \sum_{i=1}^{n}(x_i - \theta)$$

$$= \left(\sum_{i=1}^{n} x_i\right) - n\theta = 0$$

And verify it's max, not min & not better on boundary



$$\widehat{\theta} = \left(\sum_{i=1}^{n} x_i\right) / n = \overline{x}$$

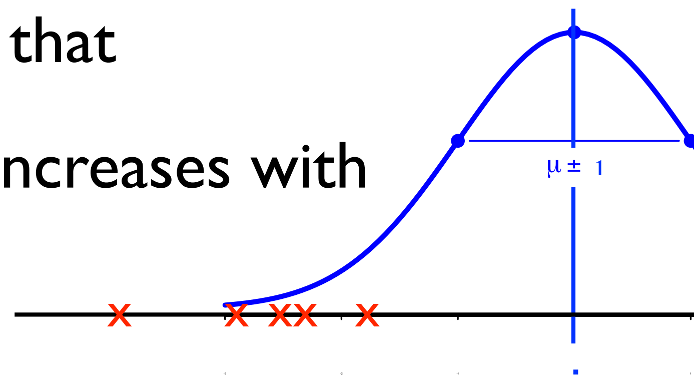
Sample mean is MLE of population mean

Hmm …, density ≠ probability

So why is "likelihood" function equal to product of *densities*?? (Prob of seeing any specific x_i is 0, right?)

a) for maximizing likelihood, we really only care about *relative* likelihoods, and density captures that

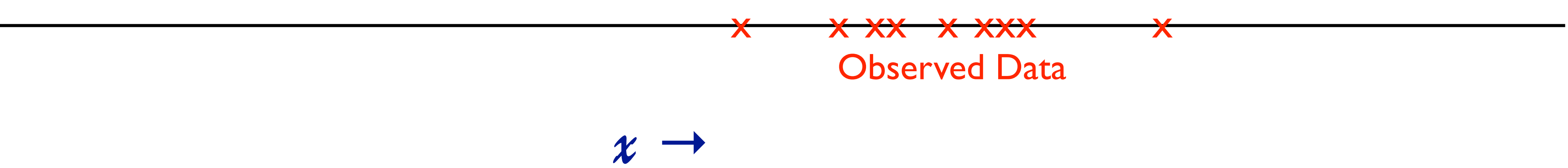
b) has desired property that likelihood increases with better fit to the model



and/or

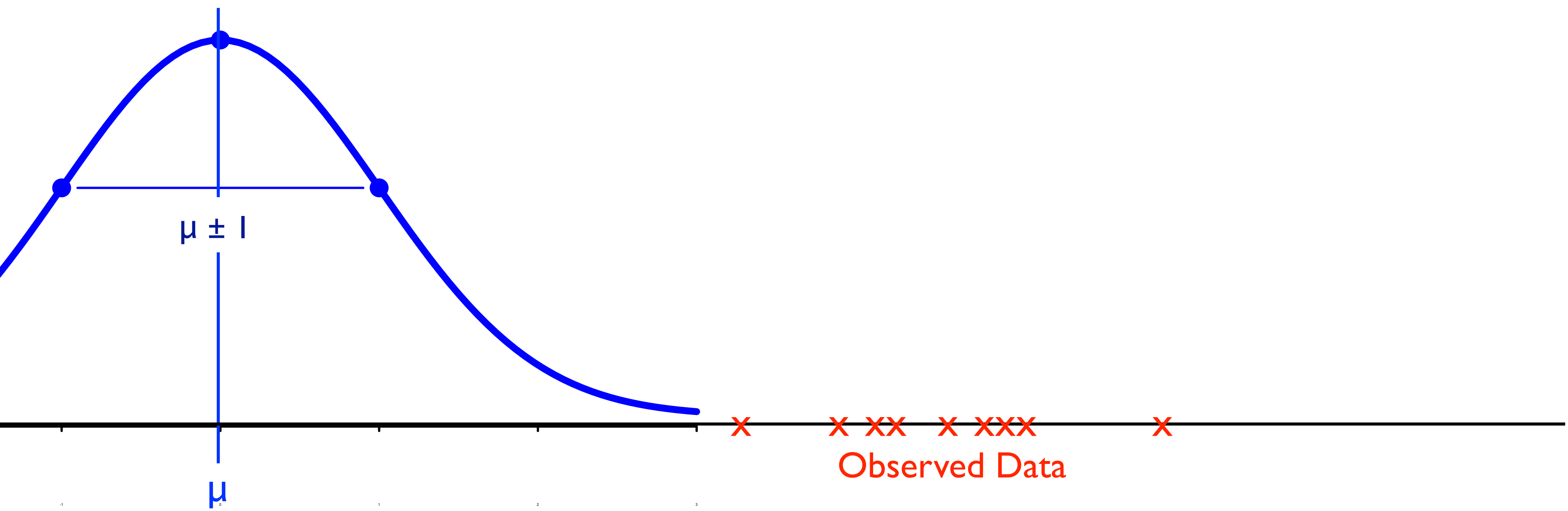
c) if density at x is $f(x)$, for any small $\delta>0$, the probability of a sample within $\pm\delta/2$ of x is $\approx \delta f(x)$, but δ is *constant* wrt θ, so it just drops out of $d/d\theta \log L(\ldots) = 0$.

Ex3: I got data; a little birdie tells me it's normal (but does *not* tell me μ, σ^2)



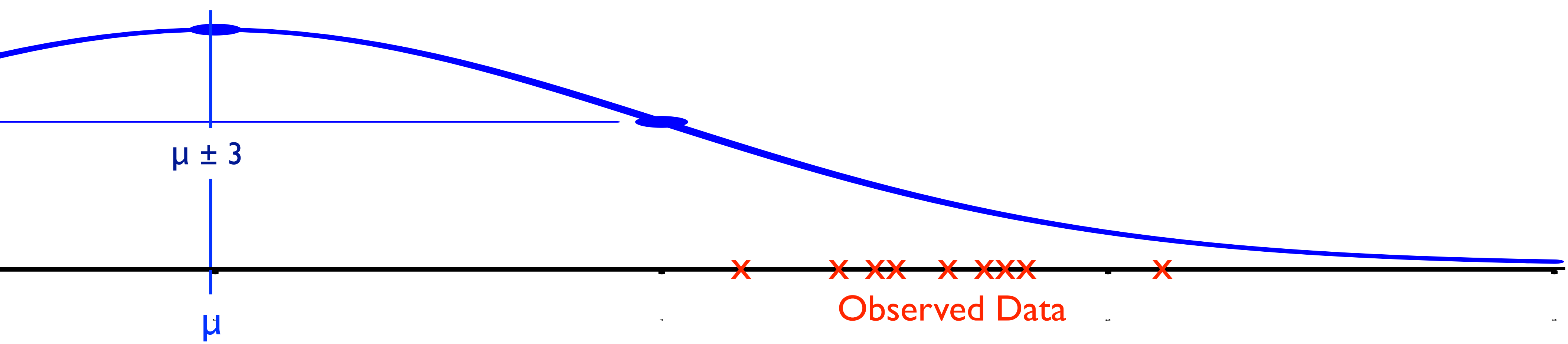
Which is more likely: (a) this?

μ, σ^2 both unknown



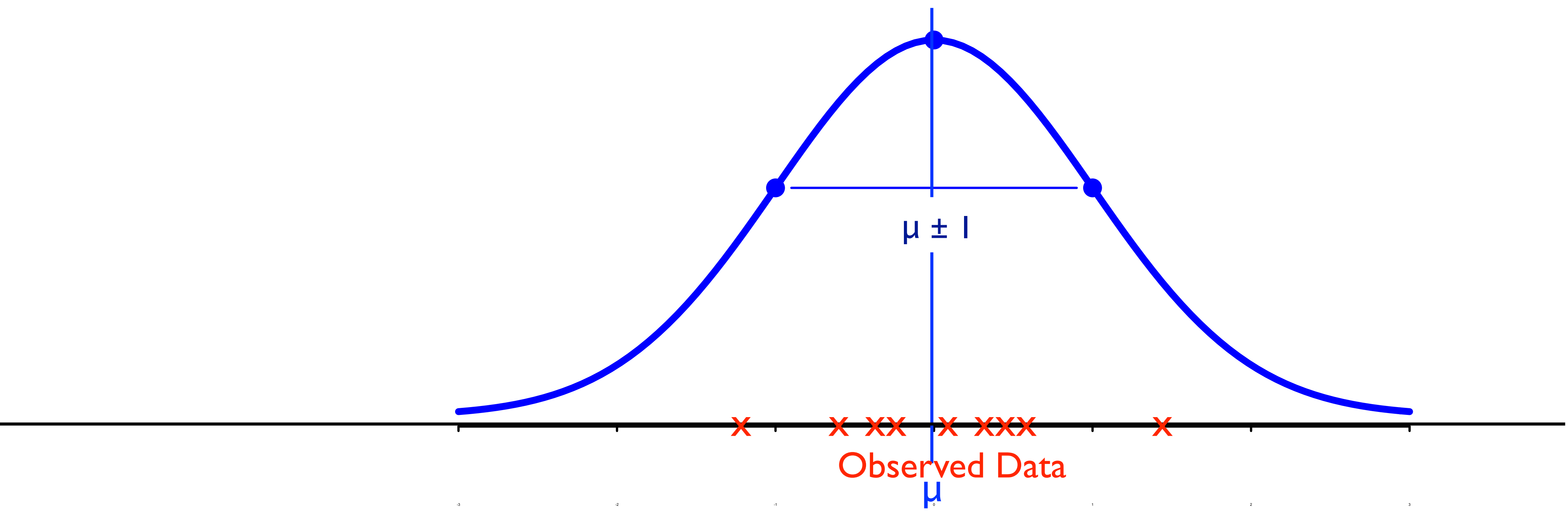
Which is more likely: (b) or this?

μ, σ^2 both unknown

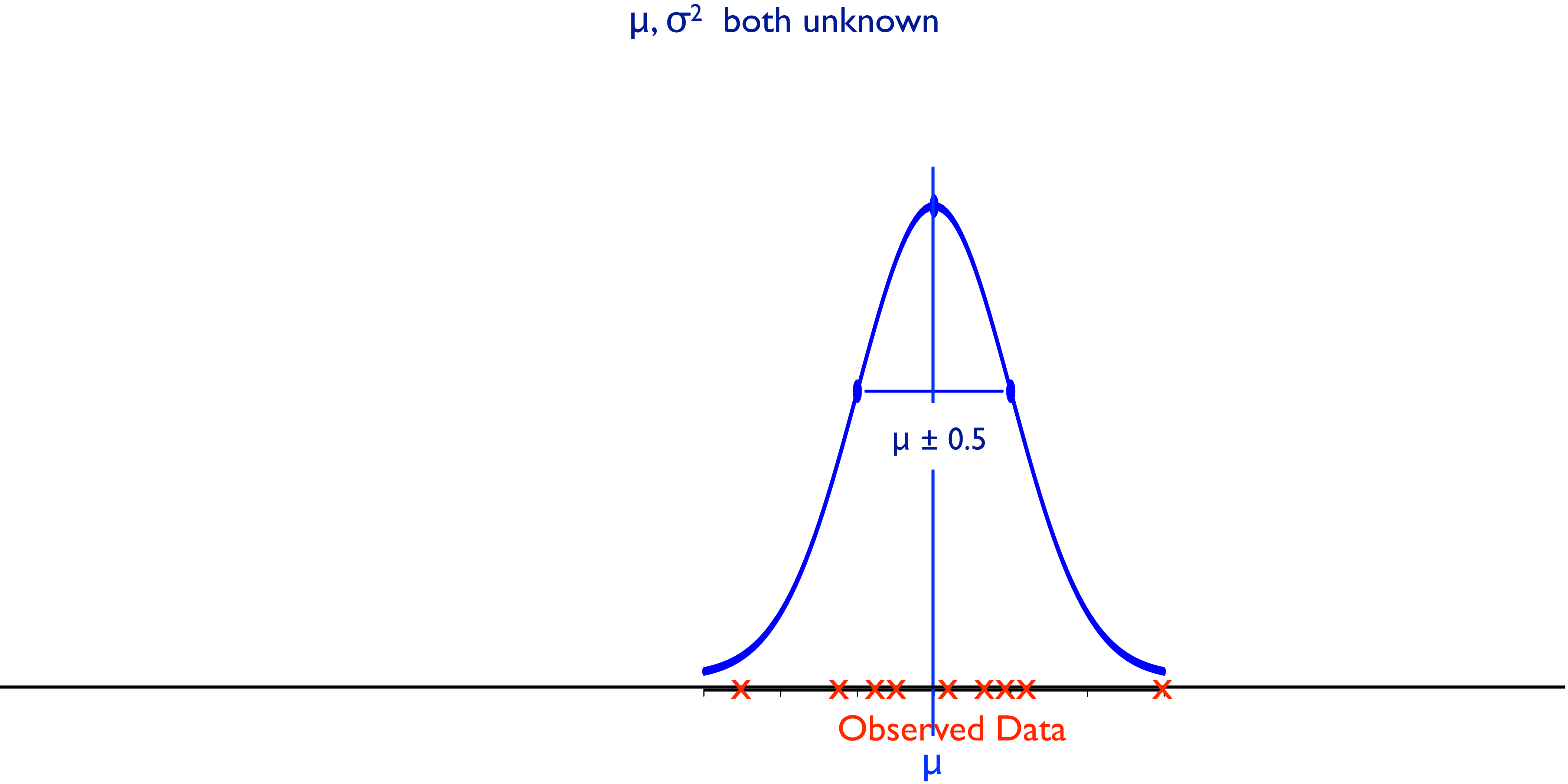


Which is more likely: (c) or this?

μ, σ^2 both unknown



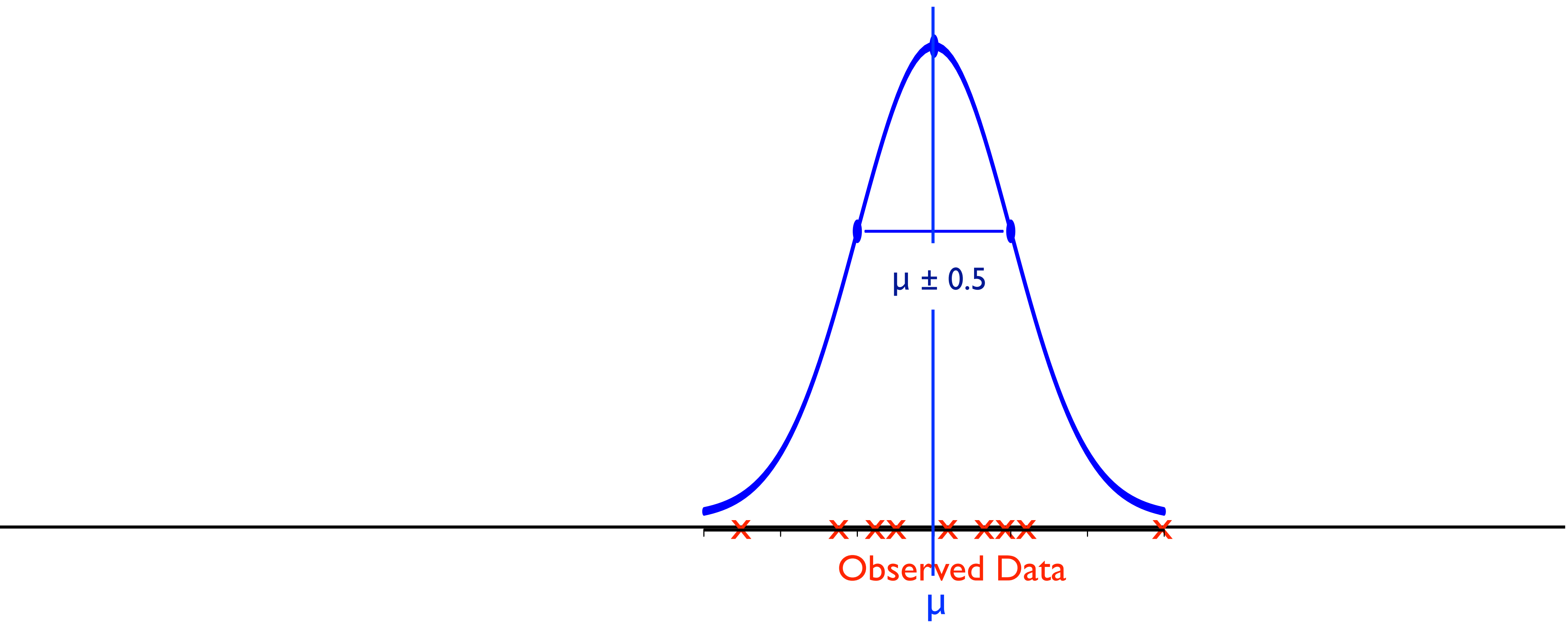
Which is more likely: (d) or *this*?



Which is more likely: (d) or *this*?

μ, σ^2 both unknown

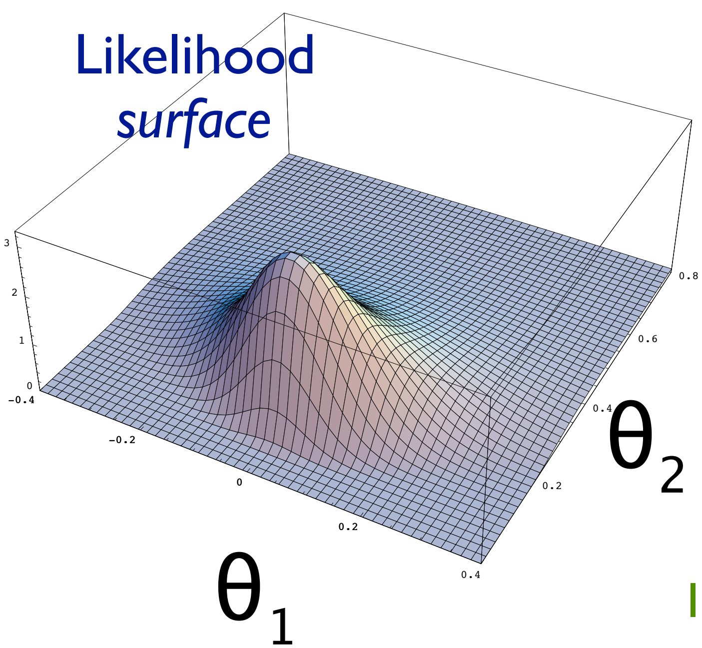
Looks good by eye, but how do I optimize my estimates of μ & σ^2 ?



Ex 3: $x_i \sim N(\mu, \sigma^2), \ \mu, \sigma^2$ both unknown

$$\ln L(x_1, x_2, \ldots, x_n | \theta_1, \theta_2) = \sum_{i=1}^{n} -\frac{1}{2} \ln(2\pi\theta_2) - \frac{(x_i - \theta_1)^2}{2\theta_2}$$

$$\frac{\partial}{\partial \theta_1} \ln L(x_1, x_2, \ldots, x_n | \theta_1, \theta_2) = \sum_{i=1}^{n} \frac{(x_i - \theta_1)}{\theta_2} = 0$$



$$\widehat{\theta}_1 = \left(\sum_{i=1}^{n} x_i \right) / n = \overline{x}$$

Sample mean is MLE of population mean, again

In general, a problem like this results in 2 equations in 2 unknowns. Easy in this case, since θ_2 drops out of the $\partial / \partial \theta_1 = 0$ equation

Ex. 3, (cont.)

$$\ln L(x_1, x_2, \ldots, x_n | \theta_1, \theta_2) = \sum_{i=1}^{n} -\frac{1}{2} \ln(2\pi\theta_2) - \frac{(x_i - \theta_1)^2}{2\theta_2}$$

$$\frac{\partial}{\partial\theta_2} \ln L(x_1, x_2, \ldots, x_n | \theta_1, \theta_2) = \sum_{i=1}^{n} -\frac{1}{2} \frac{2\pi}{2\pi\theta_2} + \frac{(x_i - \theta_1)^2}{2\theta_2^2} = 0$$

$$\widehat{\theta}_2 = \left(\sum_{i=1}^{n} (x_i - \widehat{\theta}_1)^2 \right) / n = \overline{s}^2$$

Sample variance is MLE of *population* variance

Summary

MLE is *one* way to estimate *parameters* from *data*

You choose the *form* of the model (normal, binomial, ...)

Math chooses the *value(s)* of parameter(s)

Defining the "Likelihood Function" (based on the form of the model) is often the critical step; the math/algorithms to optimize it are generic

- Often simply $(d/d\theta)(\log \text{Likelihood}) = 0$

Has the intuitively appealing property that the parameters maximize the *likelihood* of the observed data; basically just assumes your sample is "representative"

- Of course, unusual samples will give bad estimates (estimate normal human heights from a sample of NBA stars?) but that is an unlikely event

Often, but not always, MLE has other desirable properties like being *unbiased*, or at least *consistent*

EM

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: $\mu = 7$.

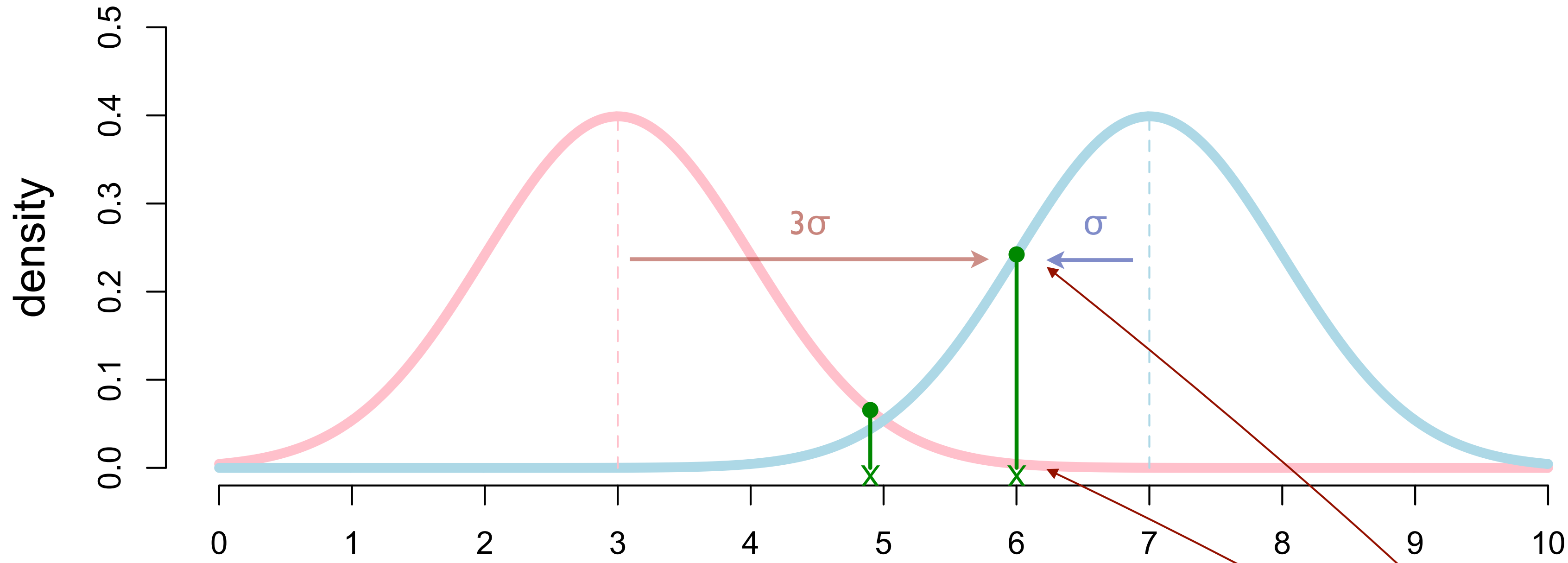
You draw one, then (without revealing color or μ) reveal a single sample $X \sim \text{Normal}(\text{mean } \mu, \sigma^2 = 1)$.

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

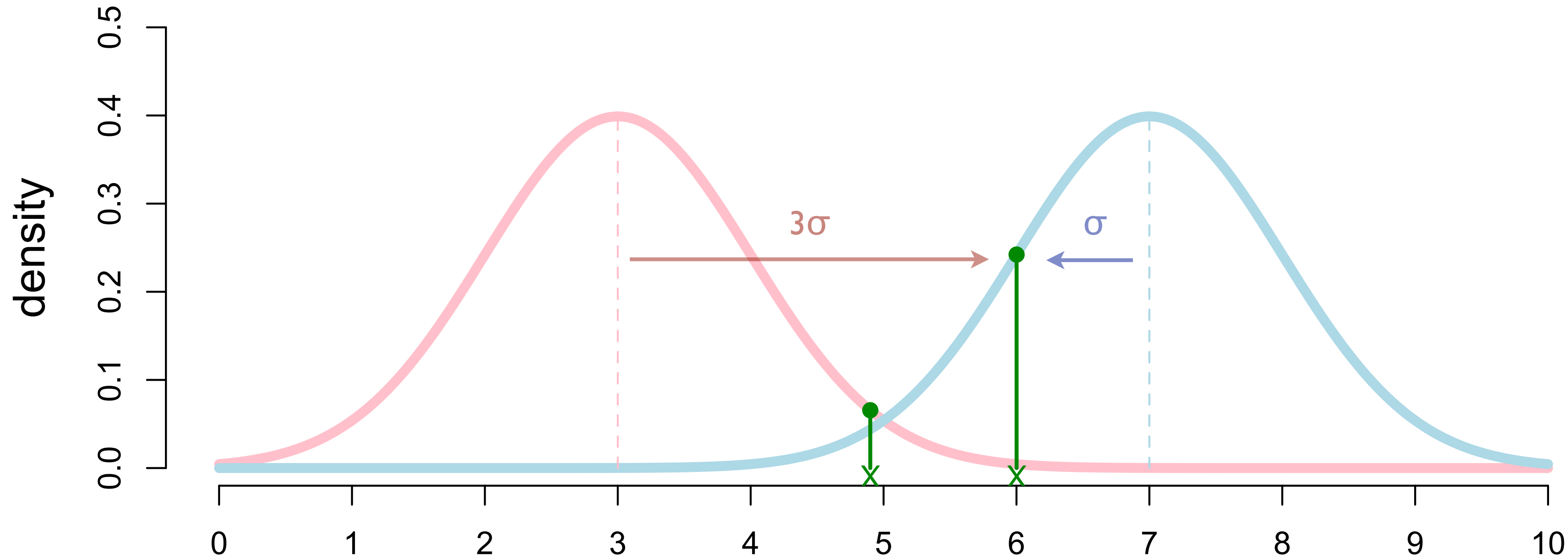
$$= \frac{0.5 P(X \approx 6 | \mu = 7)}{0.5 P(X \approx 6 | \mu = 3) + 0.5 P(X \approx 6 | \mu = 7)}$$

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

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

f = normal density

A Hat Trick



Alternate View:

f = normal density

$$\text{Posterior odds} = \text{Bayes Factor} \cdot \text{Prior odds}$$

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

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

$E[Y] = \mu$ ⟶ (first ?)

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

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

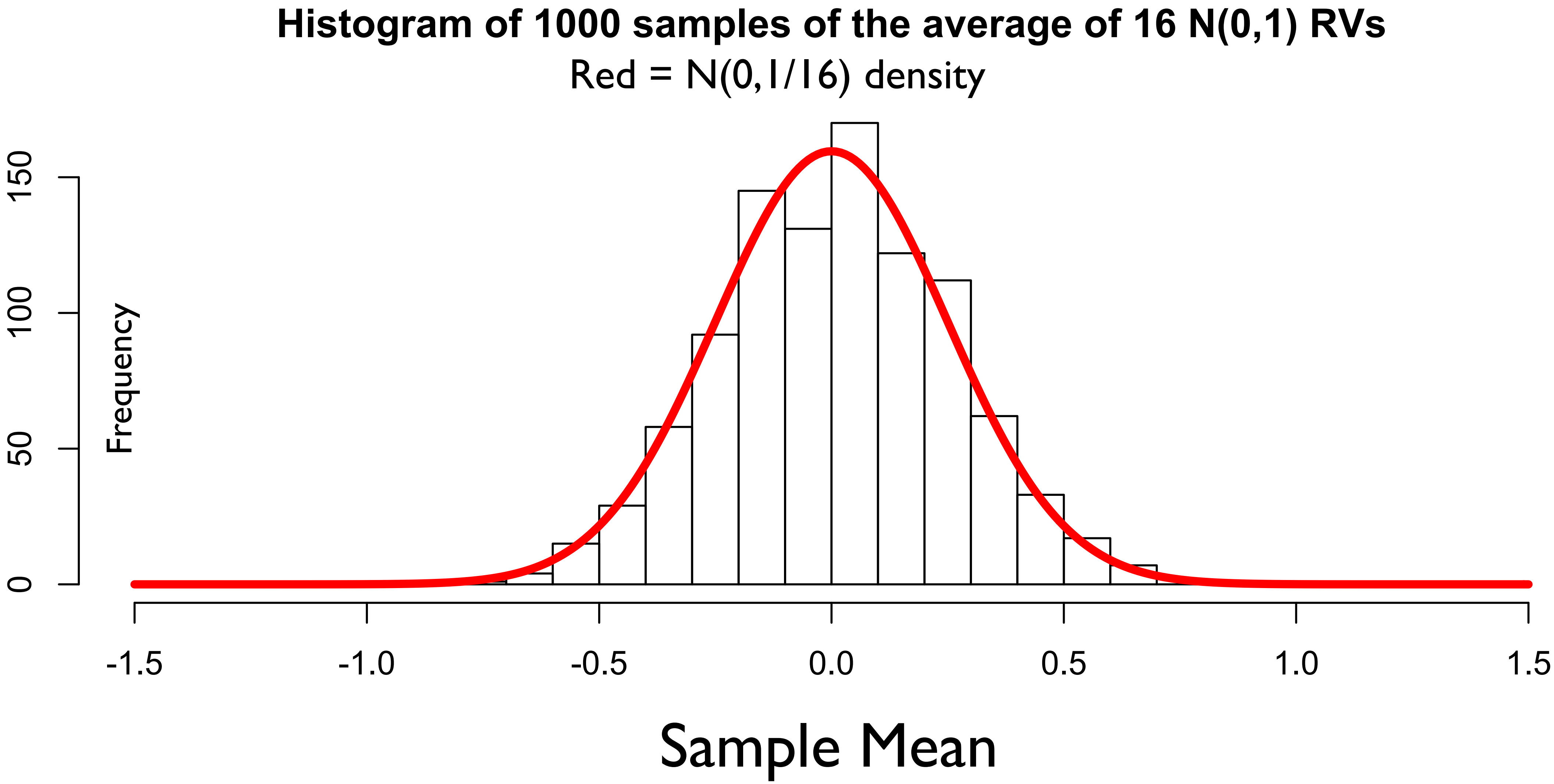
and since $0.5 = 2\ \text{sqrt}(1/16)$, we have:

"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)

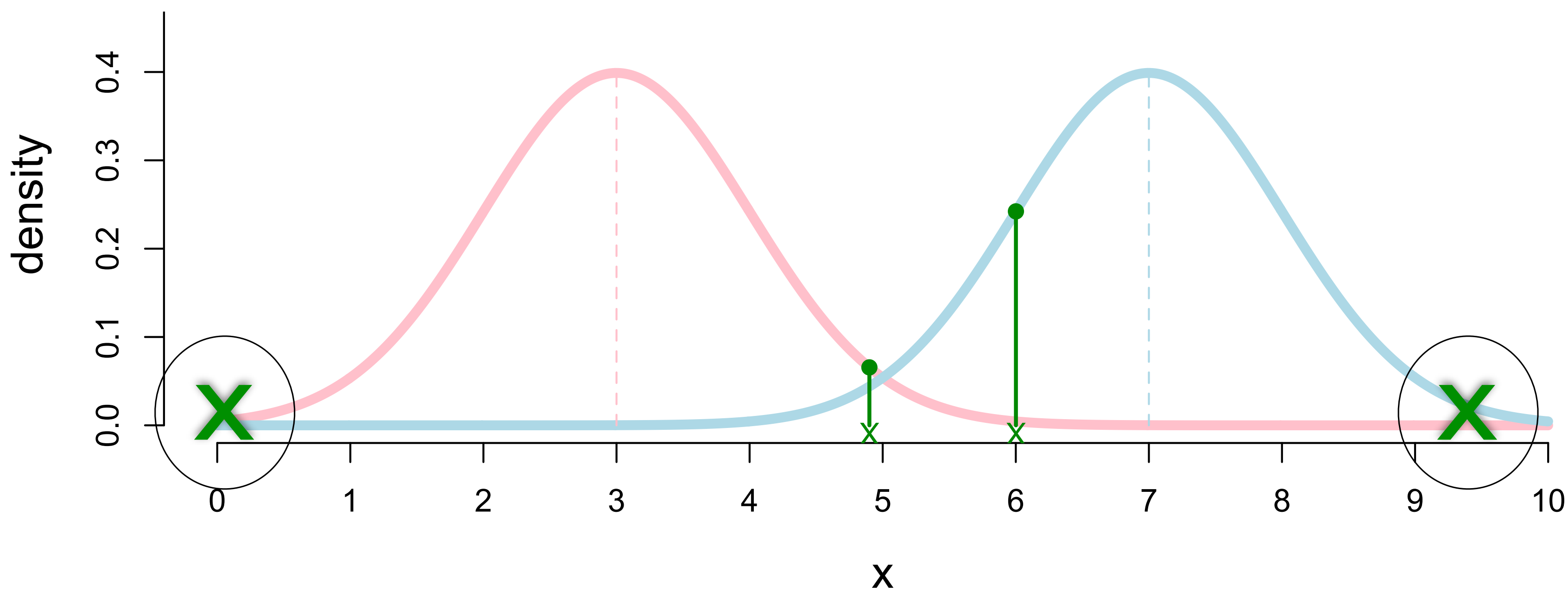

Histogram of 1000 samples of the average of 16 N(0,1) RVs
Red = N(0,1/16) density
Frequency
0
50
100
150
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
Sample Mean

Hat Trick 2 (cont.)

Note 2:

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

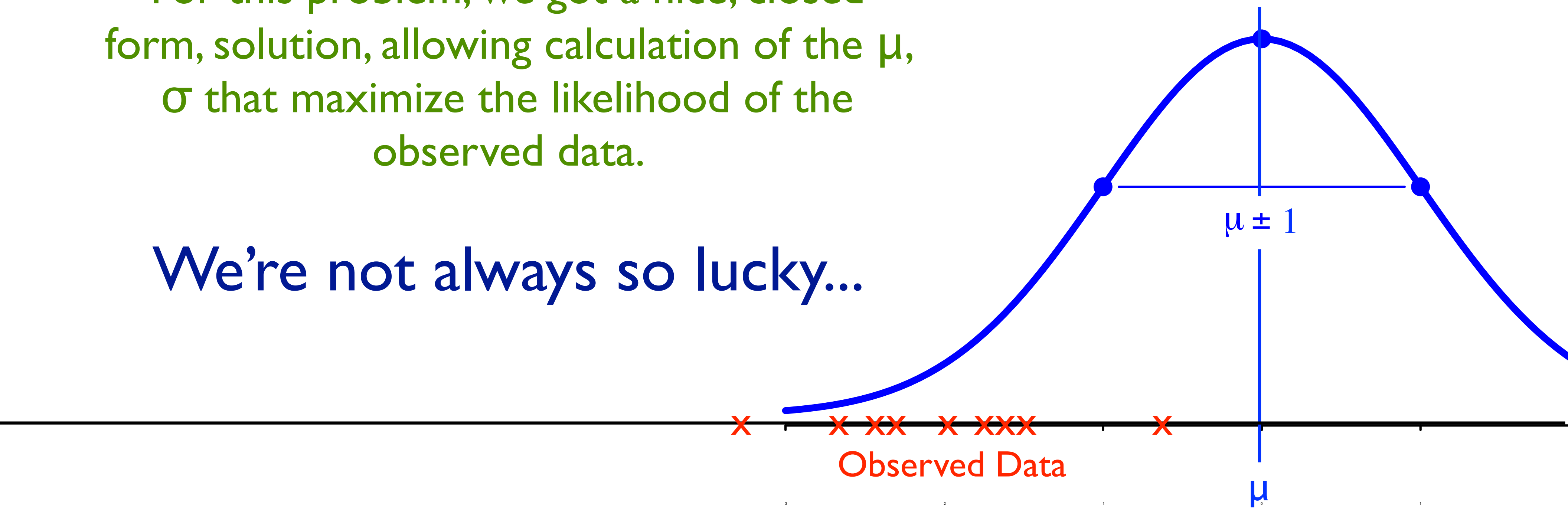
- If they were half way between means of the others?
- If they were on opposite sides of the means of the others



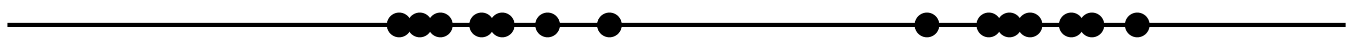
Previously:
How to estimate μ given data

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

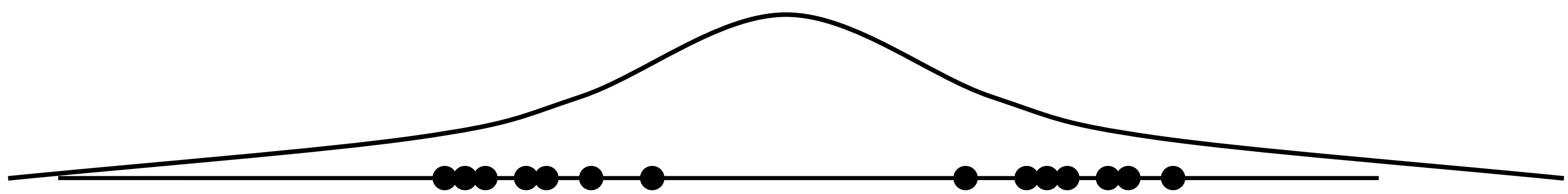
We're not always so lucky...



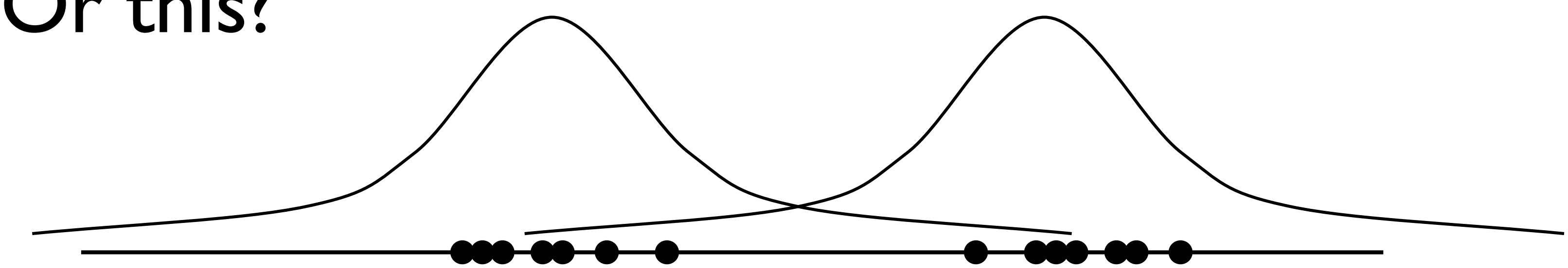
More Complex Example



This?

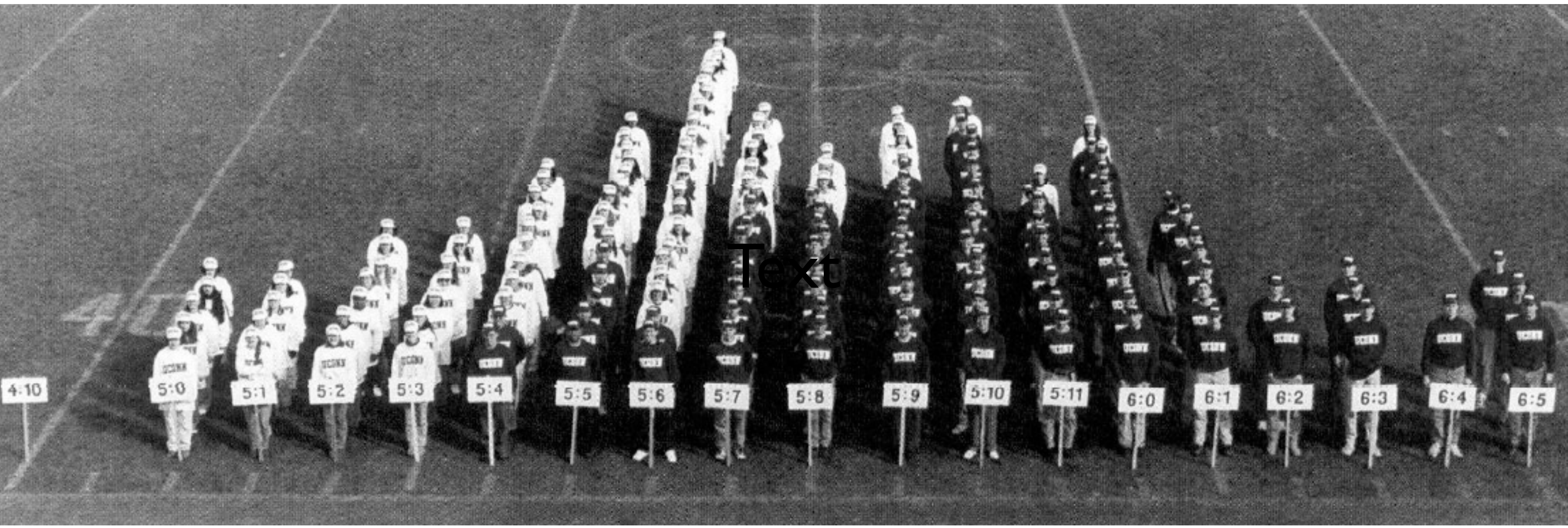


Or this?



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

A Living Histogram

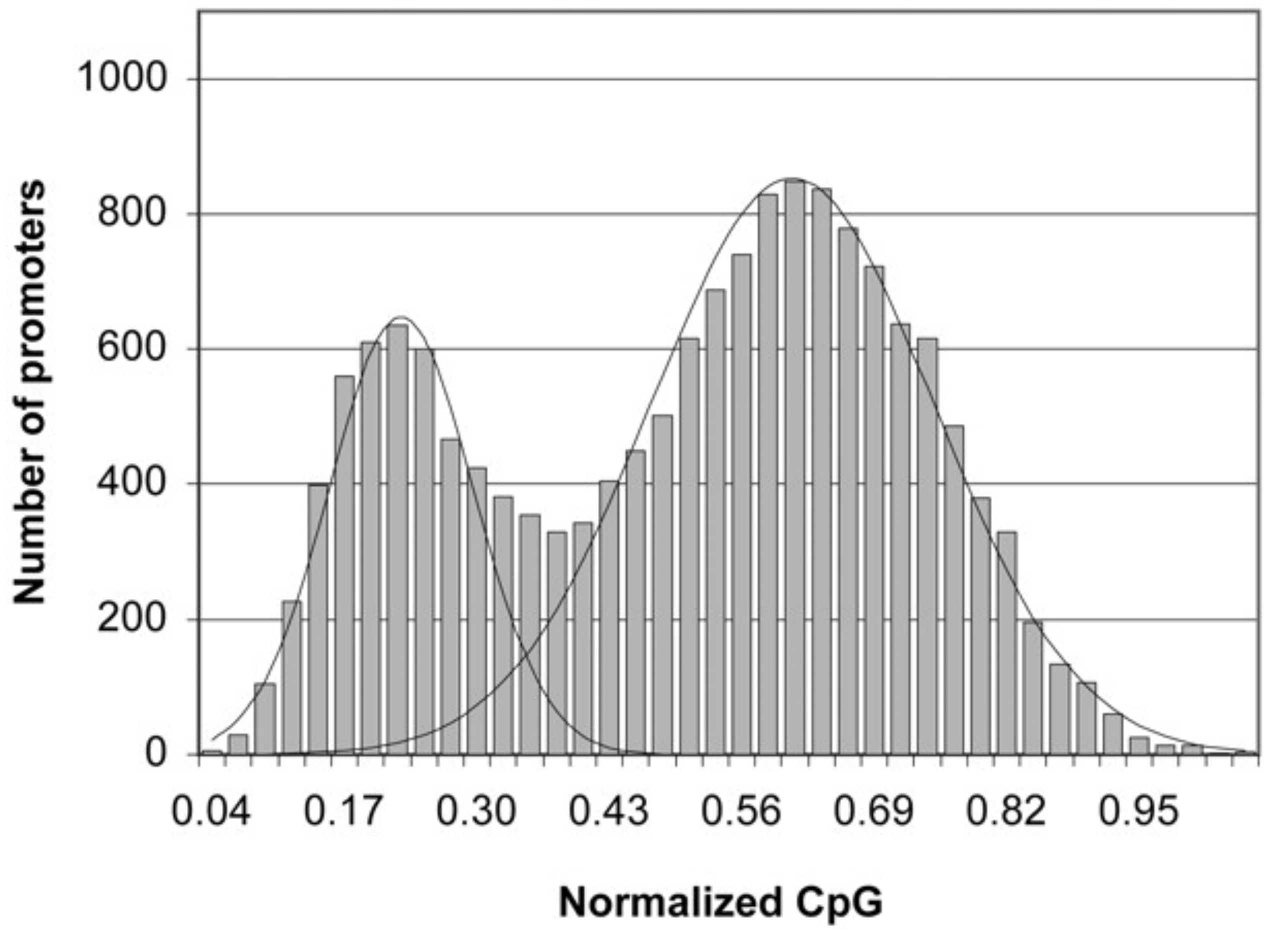


male and female genetics students, University of Connecticut in 1996

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

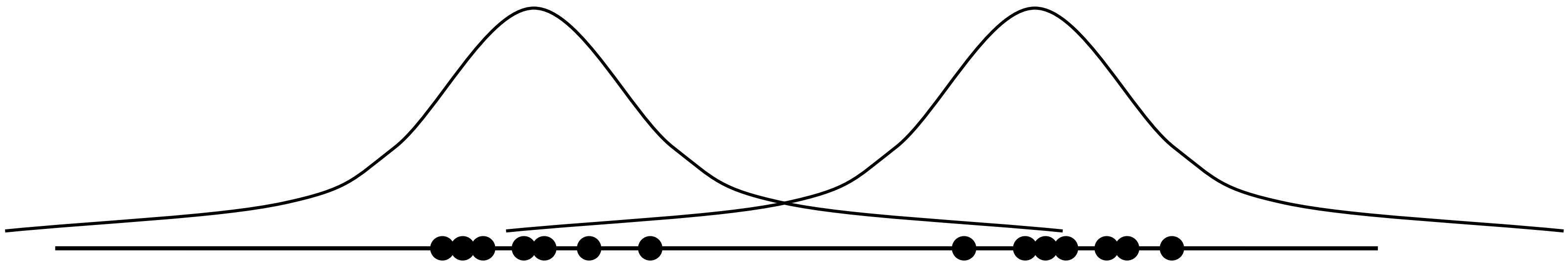
Another Real Example:

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

—together→

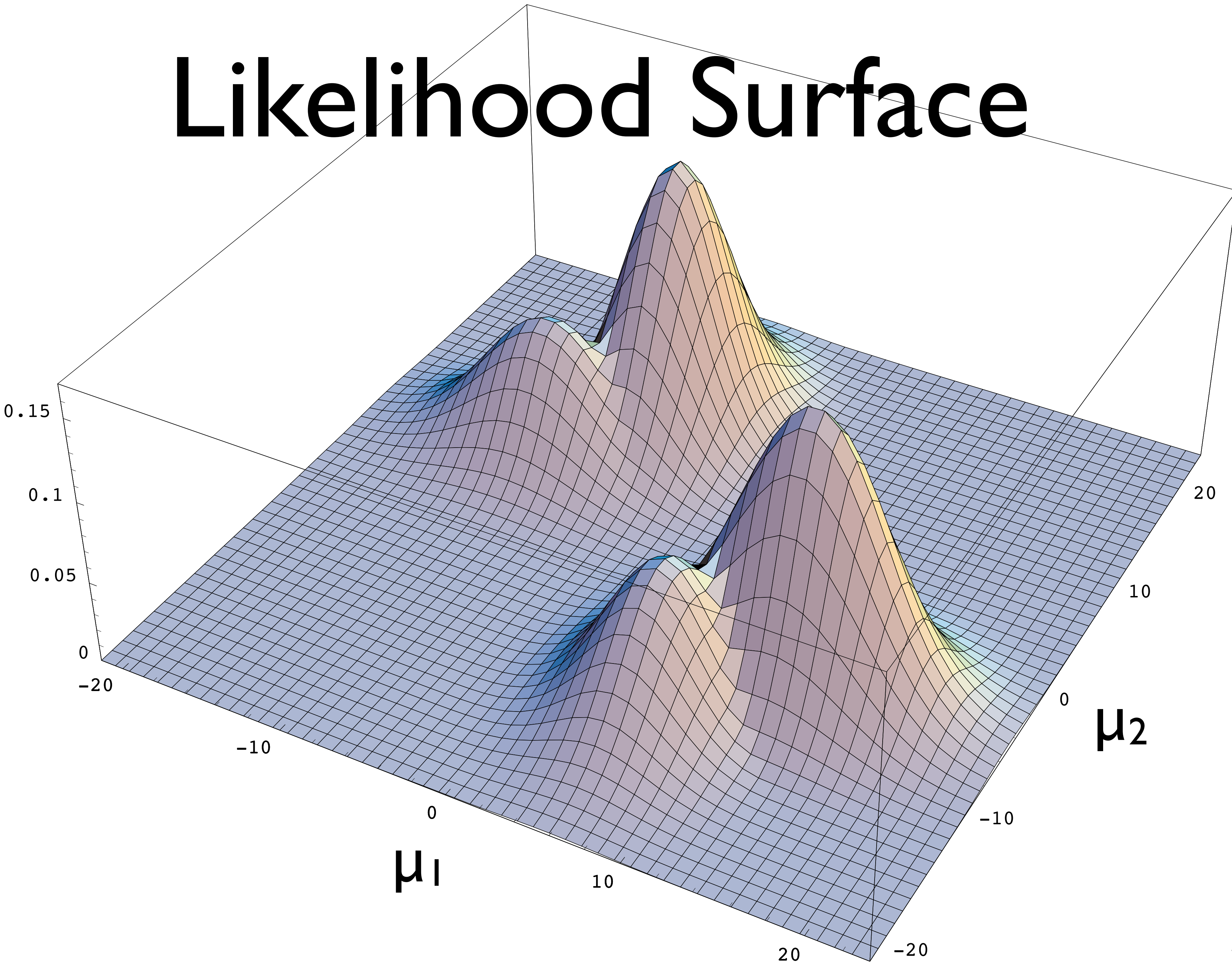
Likelihood $\boxed{\tau_1 f(x|\mu_1, \sigma_1^2) + \tau_2 f(x|\mu_2, \sigma_2^2)}$

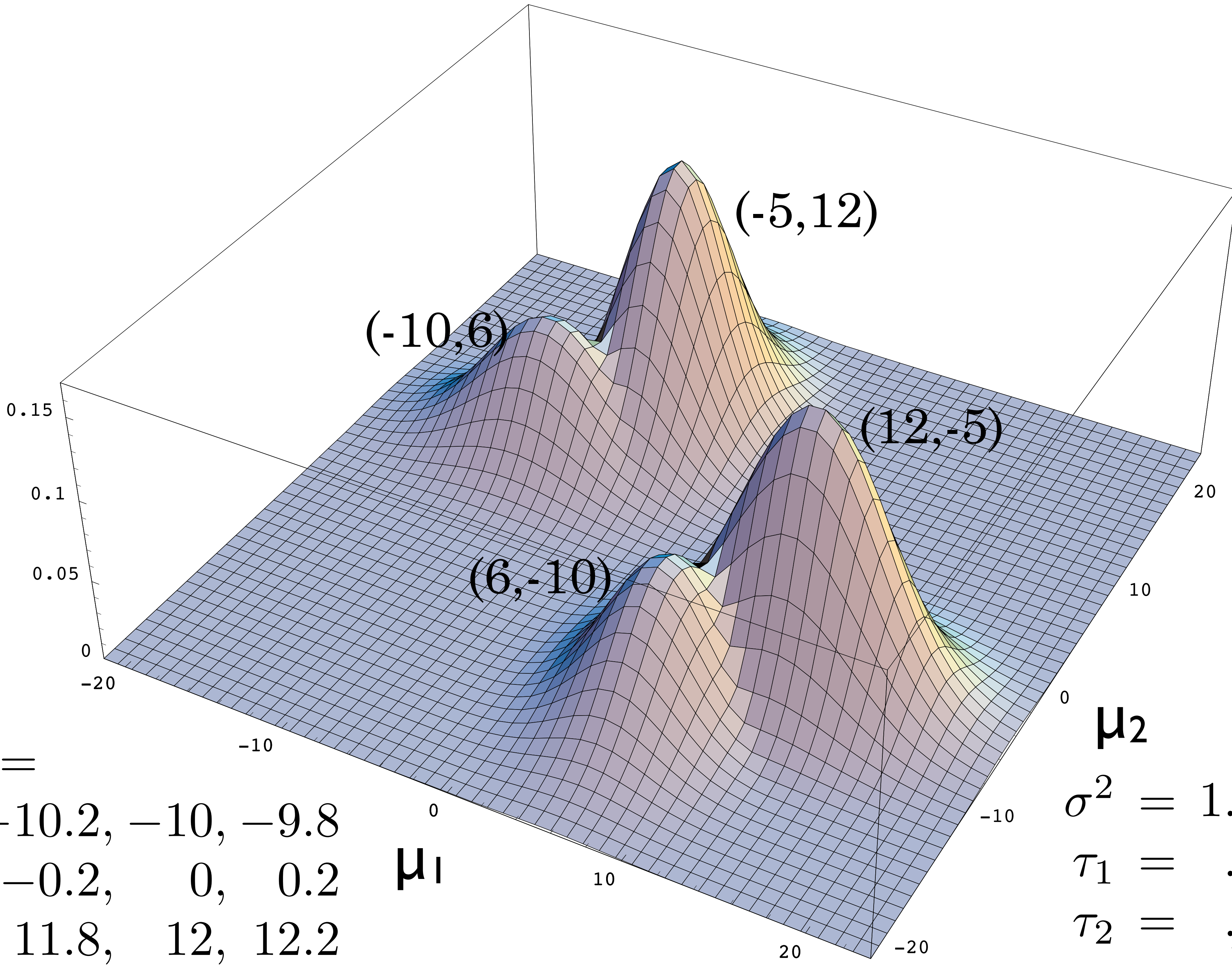
$$L(x_1, x_2, \ldots, x_n | \mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \tau_1, \tau_2)$$

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

No closed-form max

Likelihood Surface





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*?

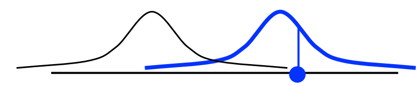
$$z_{ij} = \begin{cases} 1 & \text{if } x_i \text{ drawn from } f_j \\ 0 & \text{otherwise} \end{cases}$$

EM as Egg vs Chicken

Hat Trick 1

IF parameters θ known, could estimate z_{ij}

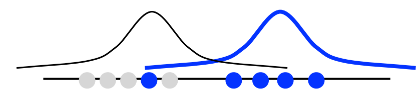
E.g., $|x_i - \mu_1|/\sigma_1 \gg |x_i - \mu_2|/\sigma_2 \Rightarrow P[z_{i1}=1] \ll P[z_{i2}=1]$



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 “EM,” 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.

Another contrast: HMM parameter estimation via “Viterbi” vs “Baum-Welch” training. In both, “hidden data” is “which state was it in at each step?” Viterbi is like E-step in classification EM: it makes a single state prediction. B-W is full EM: it captures the uncertainty in state prediction, too. For either, M-step maximizes HMM emission/transition probabilities, assuming those fixed states (Viterbi) / uncertain states (B-W).

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:

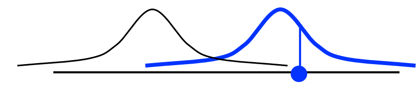
$$L(x_1, \ldots, x_n, z_{11}, z_{12}, \ldots, z_{n2} \mid \theta)$$ (complete data likelihood)

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) — $E = 0 \cdot P(0) + 1 \cdot P(1)$

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

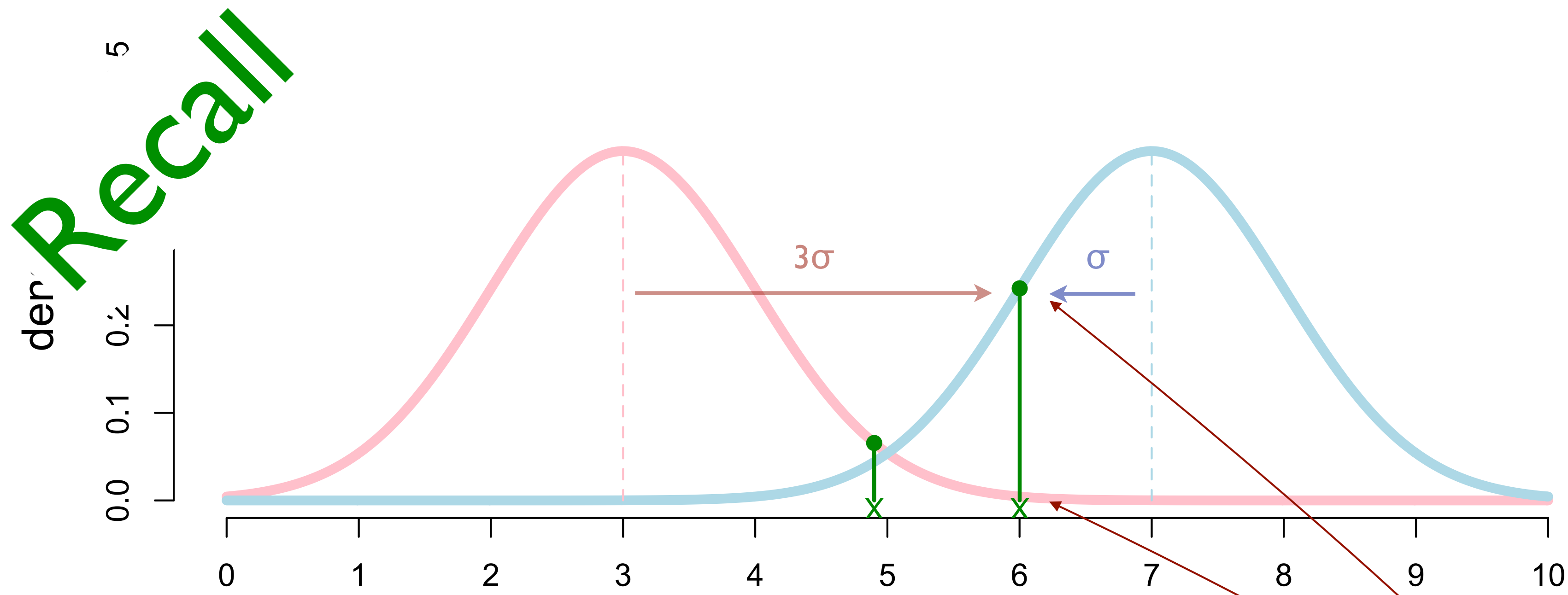
$$P(D) = P(D|A)P(A) + P(D|B)P(B)$$

$$= f_1(x_i|\theta_1)\,\tau_1 + f_2(x_i|\theta_2)\,\tau_2$$

Repeat for each x_i

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

A Hat Trick



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

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

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

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

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

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

f = normal density

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

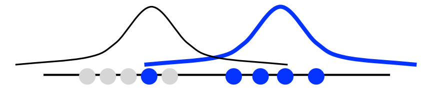
Formulas with "if's" are messy; can we blend more smoothly?
Yes, many possibilities. Idea 1:

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

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:

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

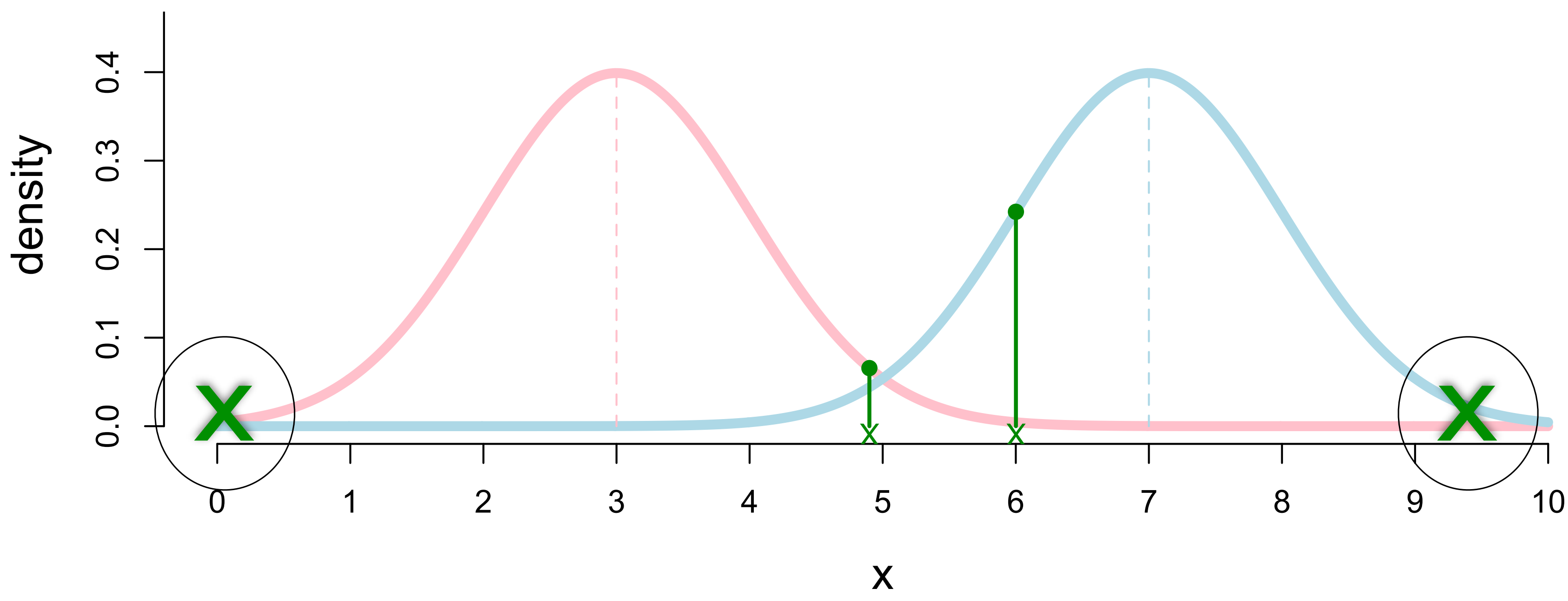
Recall

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

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

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 (DEKM sect 11.6), 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 *NP-hard* problems (including clustering, above and motif-discovery, soon)

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

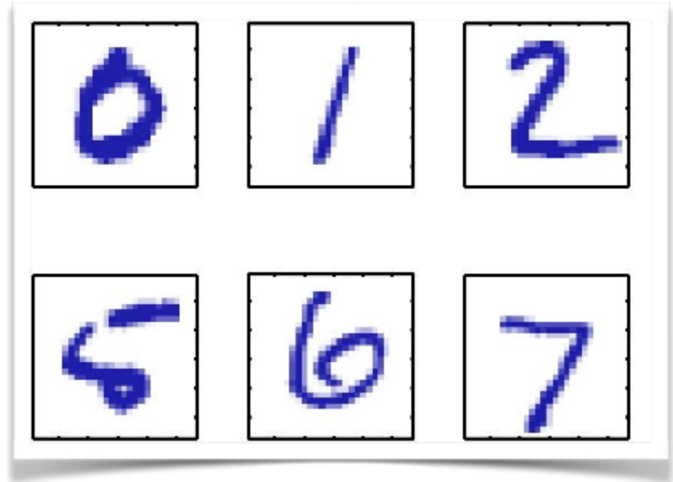
Gaussian mixture models widely used

- 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

Relative entropy

Relative Entropy

- AKA Kullback-Liebler Distance/Divergence, AKA Information Content
- Given distributions P, Q

$$H(P||Q) = \sum_{x \in \Omega} P(x) \log \frac{P(x)}{Q(x)}$$

Notes:

$$\text{Let } P(x) \log \frac{P(x)}{Q(x)} = 0 \text{ if } P(x) = 0 \text{ [since } \lim_{y \to 0} y \log y = 0]$$

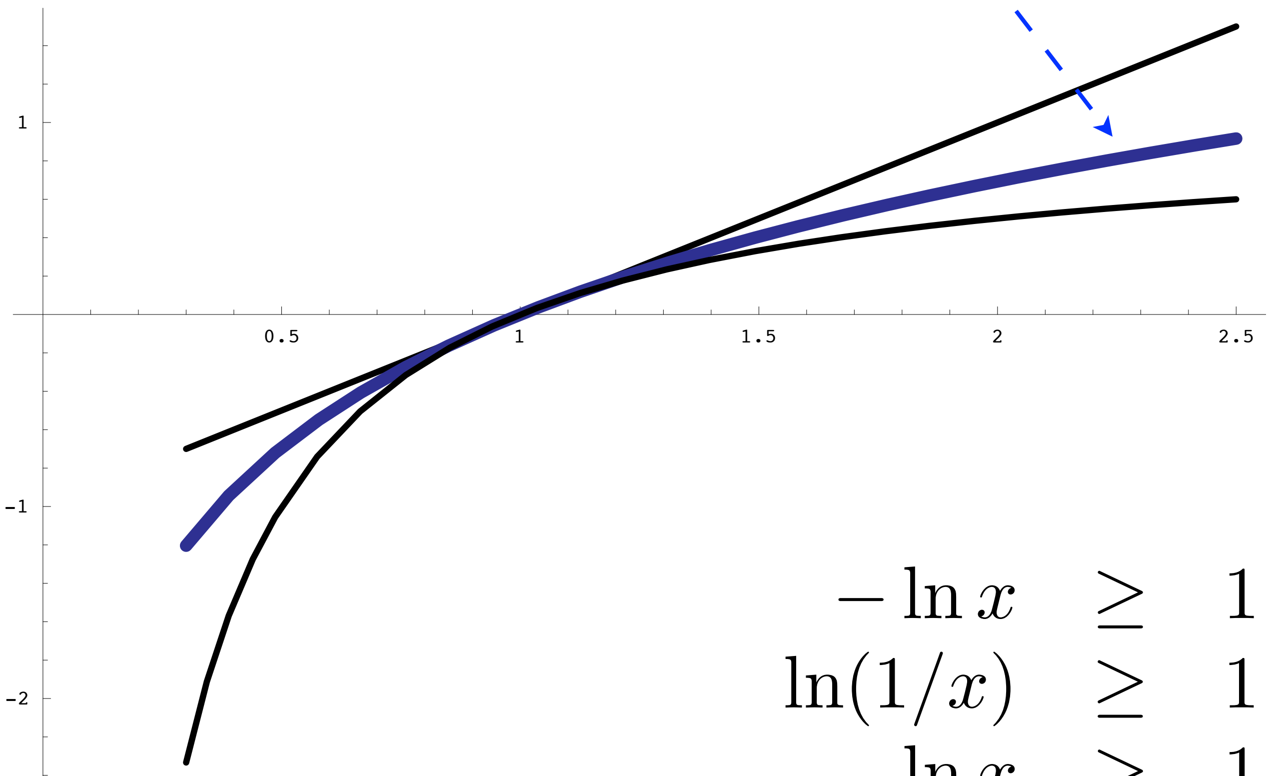
$$\text{Undefined if } 0 = Q(x) < P(x)$$

Relative Entropy

$$H(P||Q) = \sum_{x \in \Omega} P(x) \log \frac{P(x)}{Q(x)}$$

- Intuition: A quantitative measure of how much P "diverges" from Q. (Think "distance," but note it's not symmetric.)
  - If P $\approx$ Q everywhere, then log(P/Q) $\approx$ 0, so H(P||Q) $\approx$ 0
  - But as they differ more, sum is pulled above 0 (next 2 slides)
- What it means quantitatively: Suppose you sample x, but aren't sure whether you're sampling from P (call it the "null model") or from Q (the "alternate model"). Then log(P(x)/Q(x)) is the log likelihood ratio of the two models given that datum. H(P||Q) is the *expected per sample contribution to the log likelihood ratio* for discriminating between those two models.
- Exercise: if H(P||Q) = 0.1, say. Assuming Q is the correct model, how many samples would you need to confidently (say, with 1000:1 odds) reject P?

$$\ln x \quad \leq \quad x - 1$$



$$\begin{aligned} -\ln x &\geq 1 - x \\ \ln(1/x) &\geq 1 - x \\ \ln x &\geq 1 - 1/x \end{aligned}$$

Theorem: $H(P||Q) \geq 0$

$$
\begin{aligned}
H(P||Q) &= \sum_x P(x) \log \frac{P(x)}{Q(x)} \\
&\geq \sum_x P(x) \left(1 - \frac{Q(x)}{P(x)}\right) \\
&= \sum_x (P(x) - Q(x)) \\
&= \sum_x P(x) - \sum_x Q(x) \\
&= 1 - 1 \\
&= 0
\end{aligned}
$$

Idea: if P ≠ Q, then

P(x)>Q(x) ⇒ log(P(x)/Q(x))>0

and

P(y)<Q(y) ⇒ log(P(y)/Q(y))<0

Q: Can this pull H(P||Q) < 0?
A: No, as theorem shows.
Intuitive reason: sum is *weighted* by P(x), which is bigger at the positive log ratios vs the negative ones.

Furthermore: H(P||Q) = 0 if and only if P = Q
Bottom line: “bigger” means “more different”