

CSE P 527

Winter 2018

4. Maximum Likelihood Estimation and the E-M Algorithm

Outline

HW#2 Discussion

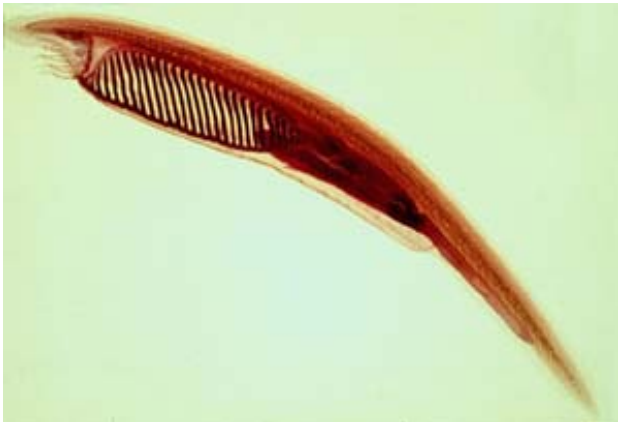
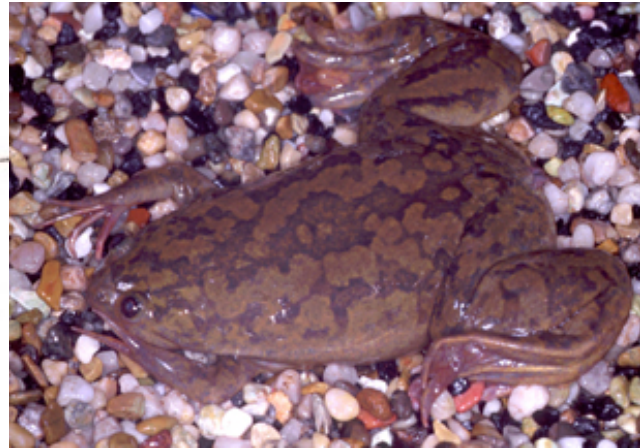
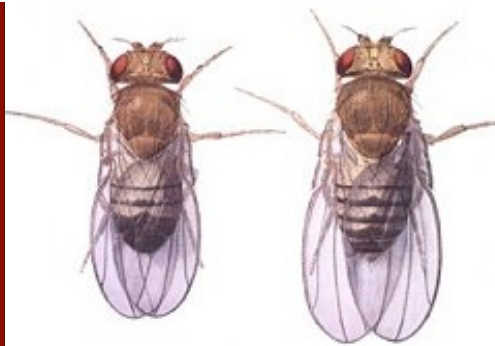
MLE: Maximum Likelihood Estimators

EM: the Expectation Maximization Algorithm

Next: Motif description & discovery

HW # 2 Discussion

	Species	Name	Description	Access-ion	score to #1
1	Homo sapiens (Human)	MYOD1_HUMAN	Myoblast determination protein 1	P15172	1709
2	Homo sapiens (Human)	TALI_HUMAN	T-cell acute lymphocytic leukemia protein 1 (TAL-1)	P17542	143
3	Mus musculus (Mouse)	MYOD1_MOUSE	Myoblast determination protein 1	P10085	1494
4	Gallus gallus (Chicken)	MYOD1_CHICK	Myoblast determination protein 1 homolog (MYOD1 homolog)	P16075	1020
5	Xenopus laevis (African clawed frog)	MYODA_XENLA	Myoblast determination protein 1 homolog A (Myogenic factor 1)	P13904	978
6	Danio rerio (Zebrafish)	MYOD1_DANRE	Myoblast determination protein 1 homolog (Myogenic factor 1)	Q90477	893
7	Branchiostoma belcheri (Amphioxus)	Q8IU24_BRABE	MyoD-related	Q8IU24	428
8	Drosophila melanogaster (Fruit fly)	MYOD_DROME	Myogenic-determination protein (Protein nautilus) (dMyd)	P22816	368
9	Caenorhabditis elegans	LIN32_CAEEL	Protein lin-32 (Abnormal cell lineage protein 32)	Q10574	118
10	Homo sapiens (Human)	SYFM_HUMAN	Phenylalanyl-tRNA synthetase, mitochondrial	O95363	56



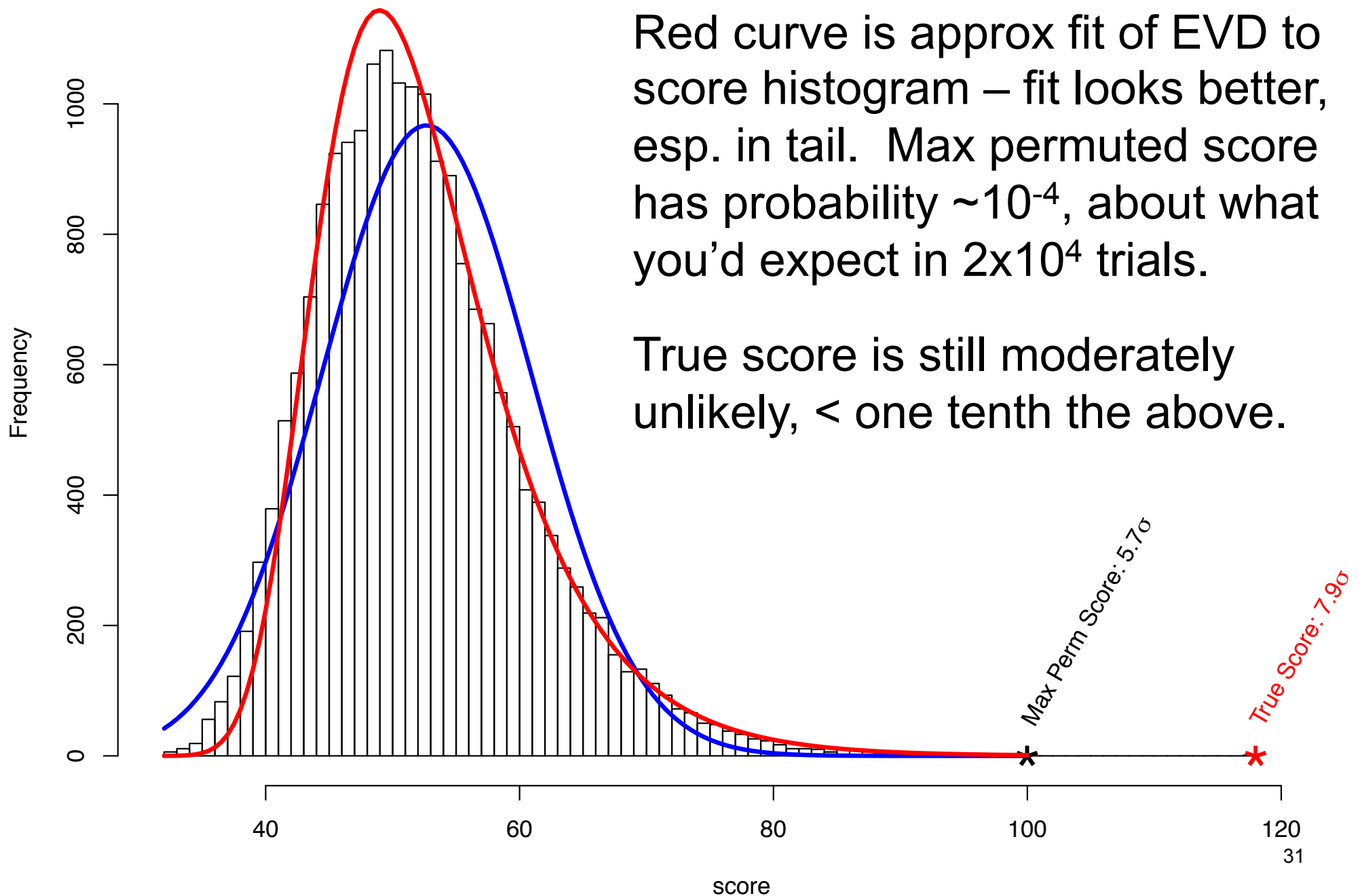
MyoD



jmol_S

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

Permutation Score Histogram vs Gaussian



Take Home

- Recognizable similarity in protein sequences over great evolutionary distance
- S-W + p-values allow useful quantification
- Similarity correlates better to “same function” than to “same species”



The Coveted
CSE P 527
Golden *Xenopus*
laevis Award



Probability Basics, I

Ex.

Ex.

Sample Space

$\{1, 2, \dots, 6\}$

\mathbb{R}

Distribution

$$p_1, \dots, p_6 \geq 0; \sum_{1 \leq i \leq 6} p_i = 1$$

$$f(x) \geq 0; \int_{\mathbb{R}} f(x) dx = 1$$

e.g.

$$p_1 = \dots = p_6 = 1/6$$

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



pdf, not
probability

Probability Basics, II

Ex.

Ex.

Expectation

$$E(g) = \sum_{1 \leq i \leq 6} g(i)p_i$$

$$E(g) = \int_{\mathbb{R}} g(x)f(x)dx$$

Population

mean

$$\mu = \sum_{1 \leq i \leq 6} ip_i$$

$$\mu = \int_{\mathbb{R}} xf(x)dx$$

variance

$$\sigma^2 = \sum_{1 \leq i \leq 6} (i - \mu)^2 p_i$$

$$\sigma^2 = \int_{\mathbb{R}} (x - \mu)^2 f(x)dx$$

Sample

mean

$$\bar{x} = \sum_{1 \leq i \leq n} x_i/n$$

variance

$$\bar{s}^2 = \sum_{1 \leq i \leq n} (x_i - \bar{x})^2/n$$

Learning From Data: MLE

Maximum Likelihood Estimators

Parameter Estimation

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

Goal: estimate θ .

Not formally “conditional probability,”
but the notation is convenient...

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

$\theta =$ probability of Heads

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

Likelihood

(For *Discrete* Distributions)

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

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

$$\text{E.g., } \sum_x P(x | \theta) = 1$$

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

E.g., $\sum_{\theta} P(x | \theta)$ can be anything; *relative* values are the focus.

E.g., if θ = prob of heads in a sequence of coin flips then

$$P(\text{HHTHH} | .6) > P(\text{HHTHH} | .5),$$

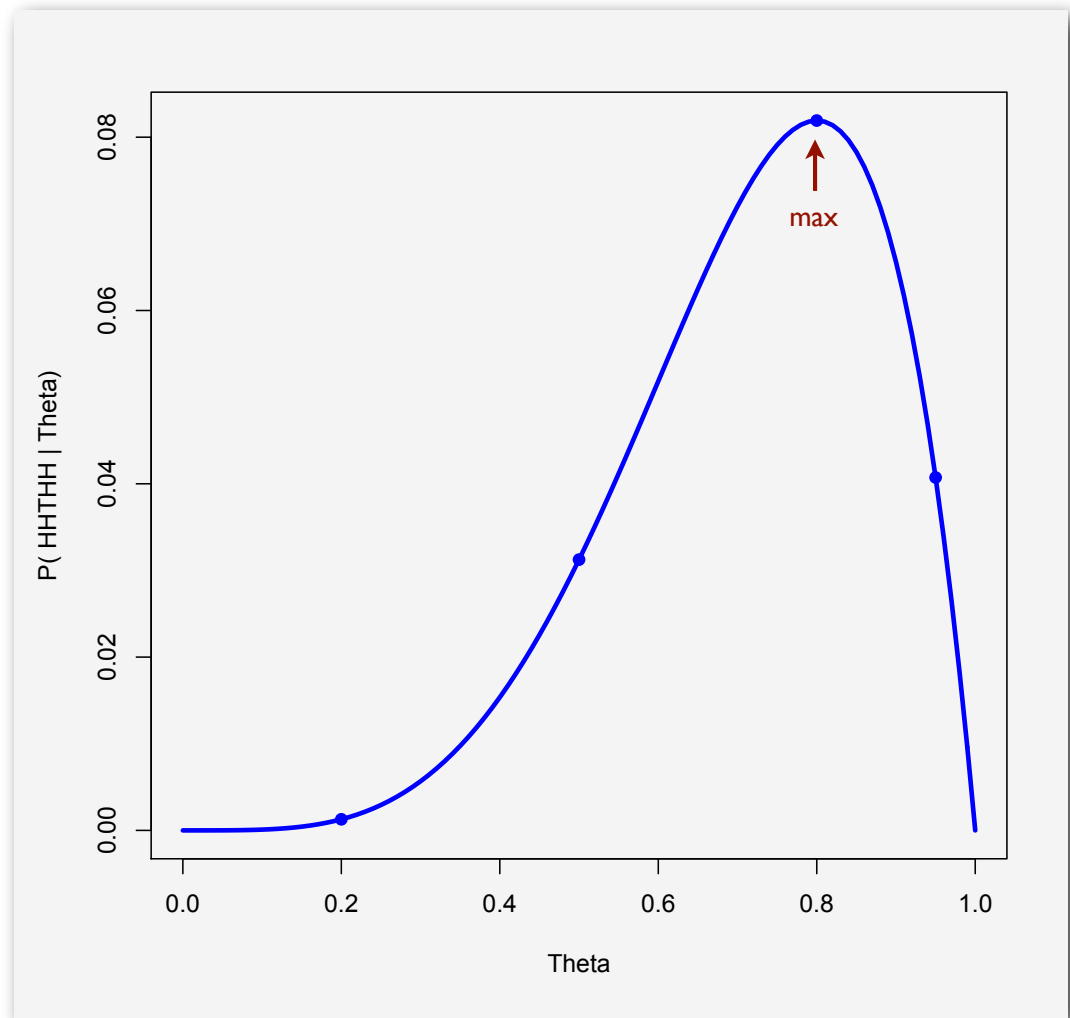
I.e., event HHTHH is *more likely* when $\theta = .6$ than $\theta = .5$

And **what θ make HHTHH *most likely*?**

Likelihood Function

$P(\text{HHTHH} \mid \theta)$:
Probability of HHTHH,
given $P(H) = \theta$:

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

(For *Discrete* Distributions)

One (of many) approaches to param. est.

Likelihood of (indp) observations x_1, x_2, \dots, x_n

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

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

(*) In general, (discrete) likelihood is the *joint* pmf; product form follows from independence

Example I

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

$$L(x_1, x_2, \dots, x_n \mid \theta) = (1 - \theta)^{n_0} \theta^{n_1}$$

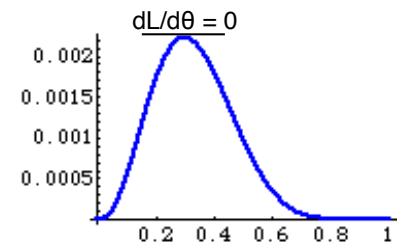
$$\log L(x_1, x_2, \dots, x_n \mid \theta) = n_0 \log(1 - \theta) + n_1 \log \theta$$

$$\frac{\partial}{\partial \theta} \log L(x_1, x_2, \dots, x_n \mid \theta) = \frac{-n_0}{1 - \theta} + \frac{n_1}{\theta}$$

Setting to zero and solving:

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

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



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

Likelihood

(For *Continuous* Distributions)

$Pr(\text{any specific } x_i) = 0$, so “likelihood = probability” won’t work. Defn: “likelihood” of x_1, \dots, x_n is their *joint density*; = (by indep) product of their *marginal densities*. (As usual, swap *density* for *pmf*.) Why sensible:

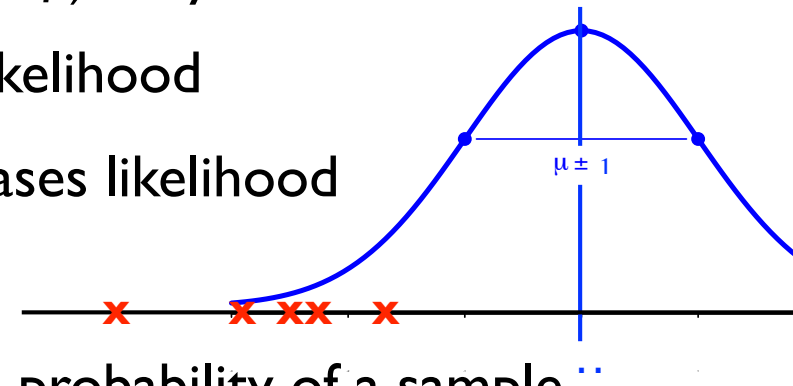
a) density captures all that matters: *relative* likelihood

b) desirable property: better model fit increases likelihood

and

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 $\approx \delta f(x)$, so density really is capturing probability, and δ is *constant* wrt θ , so it just drops out of $d/d\theta \log L(\dots) = 0$.

Otherwise, MLE is just like discrete case: get likelihood, $\frac{\partial}{\partial \theta} \log L(\vec{x} | \theta) = 0$



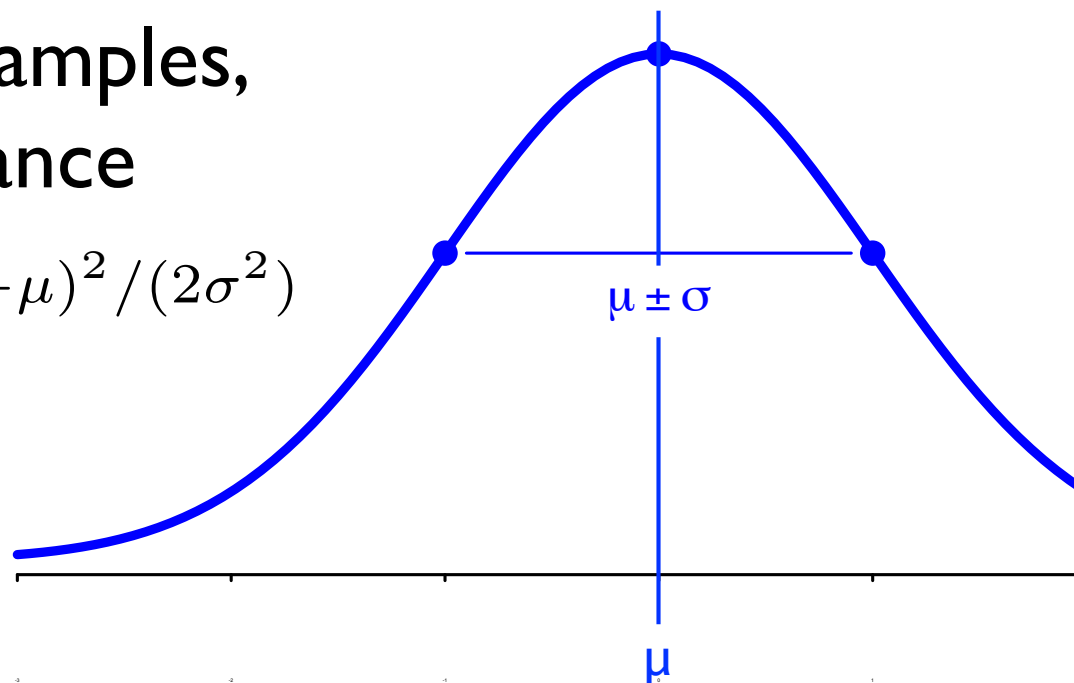
Parameter Estimation

Given: indep samples x_1, x_2, \dots, 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 $\sigma^2 = 1$

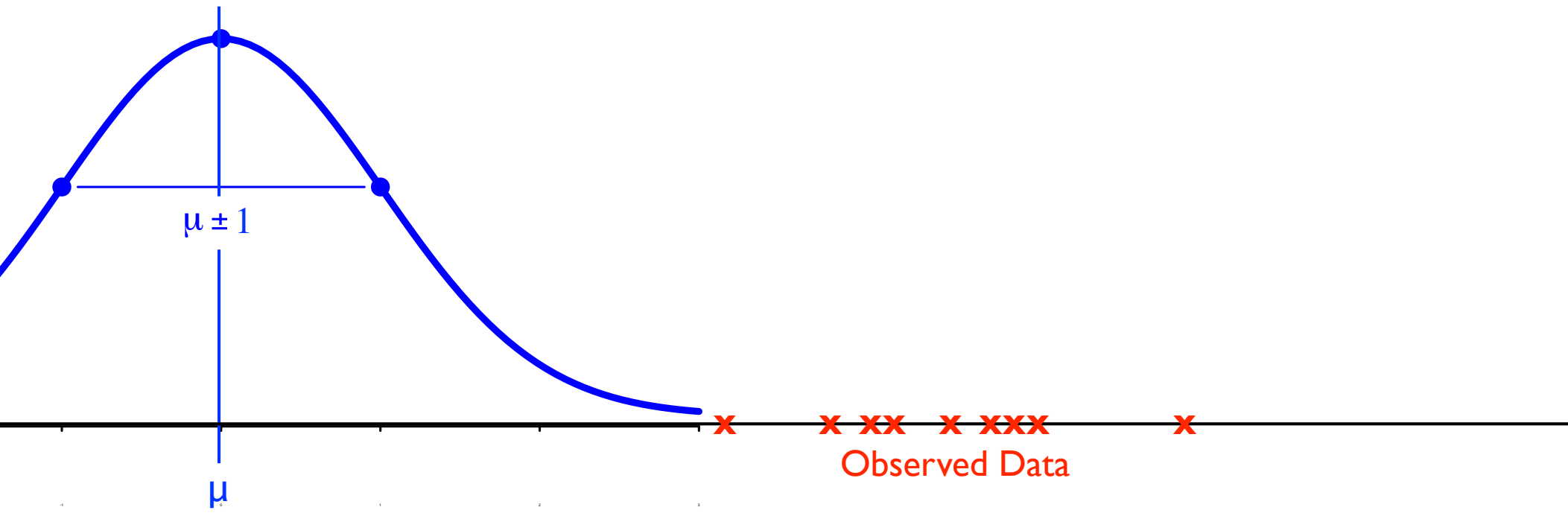


Observed Data

$x \rightarrow$

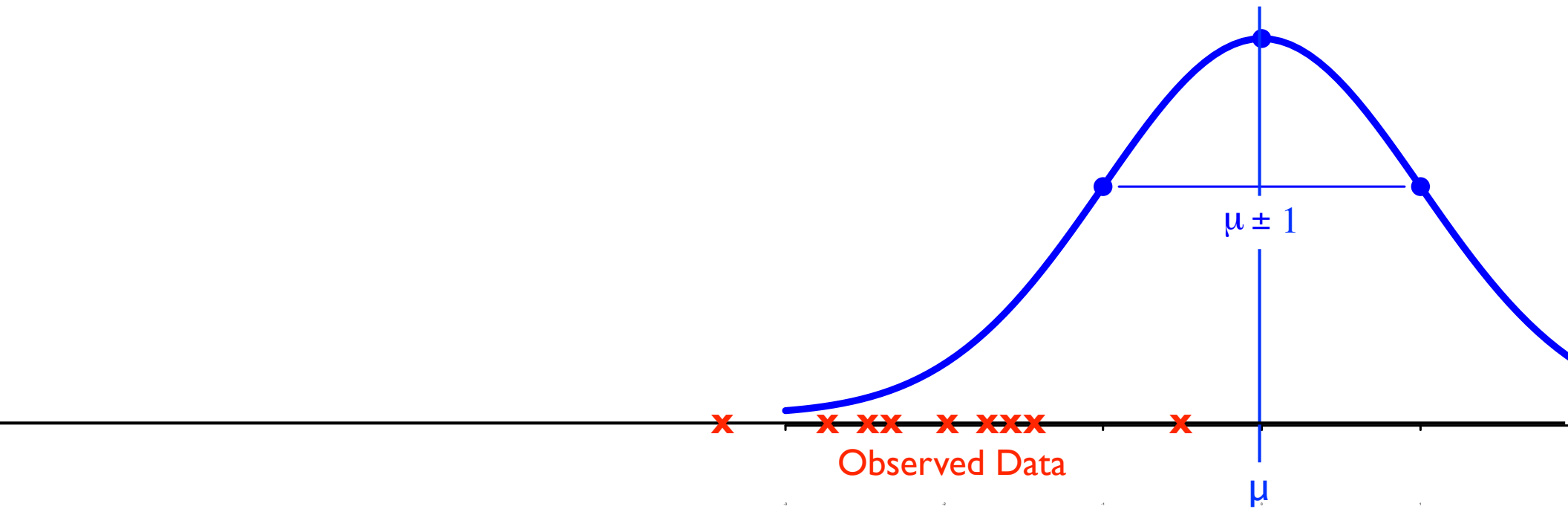
Which is more likely: (a) this?

μ unknown, $\sigma^2 = 1$



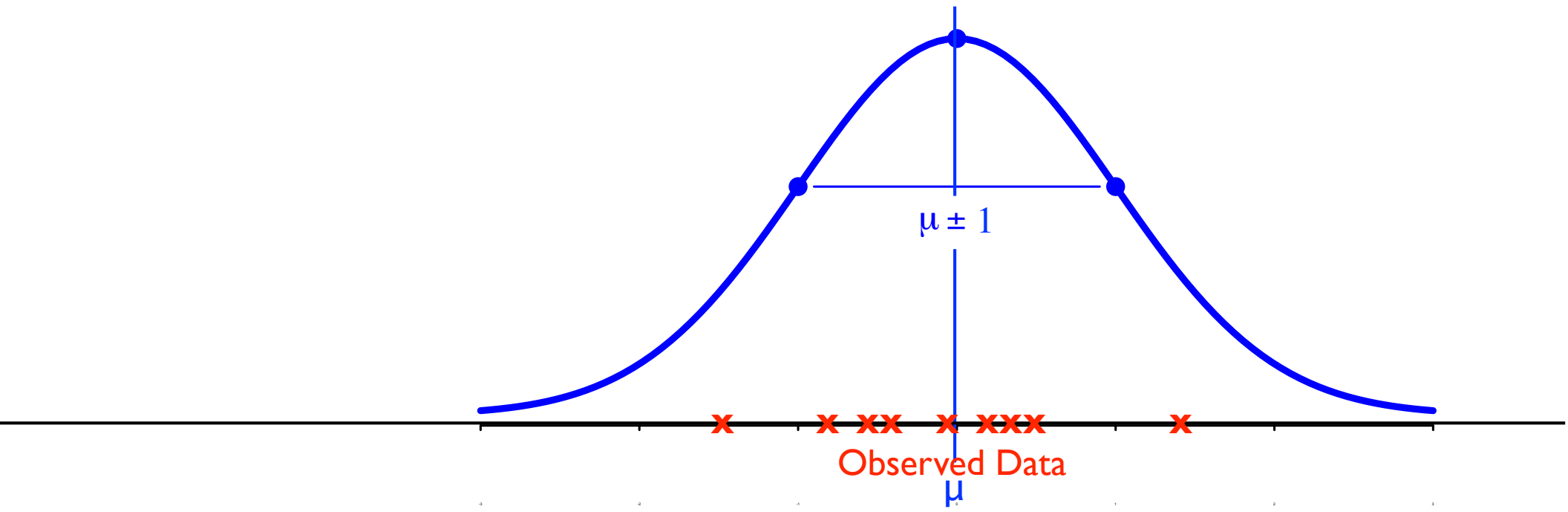
Which is more likely: (b) or this?

μ unknown, $\sigma^2 = 1$



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

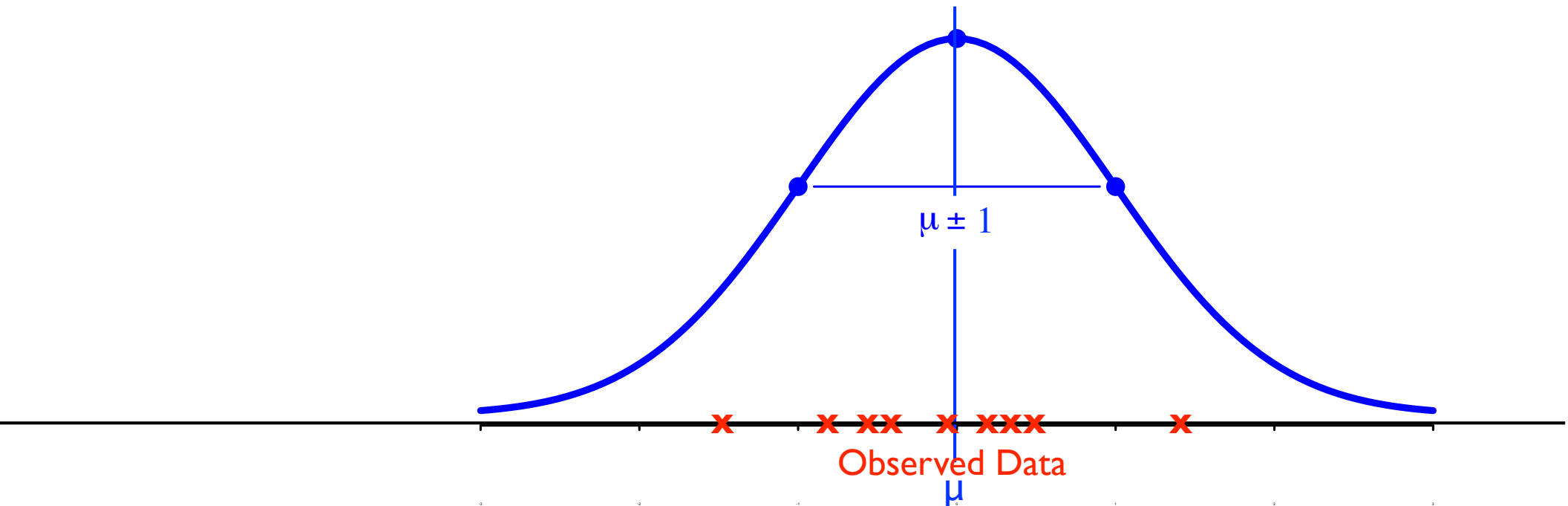
μ unknown, $\sigma^2 = 1$



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 ?



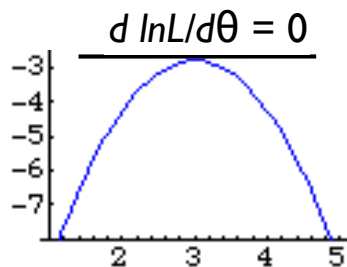
Ex. 2: $x_i \sim N(\mu, \sigma^2)$, $\sigma^2 = 1$, μ unknown

$$L(x_1, x_2, \dots, x_n | \theta) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi}} e^{-(x_i - \theta)^2 / 2} \quad \leftarrow \text{product of densities}$$

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

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

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



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

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

Sample mean is MLE of
population mean

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

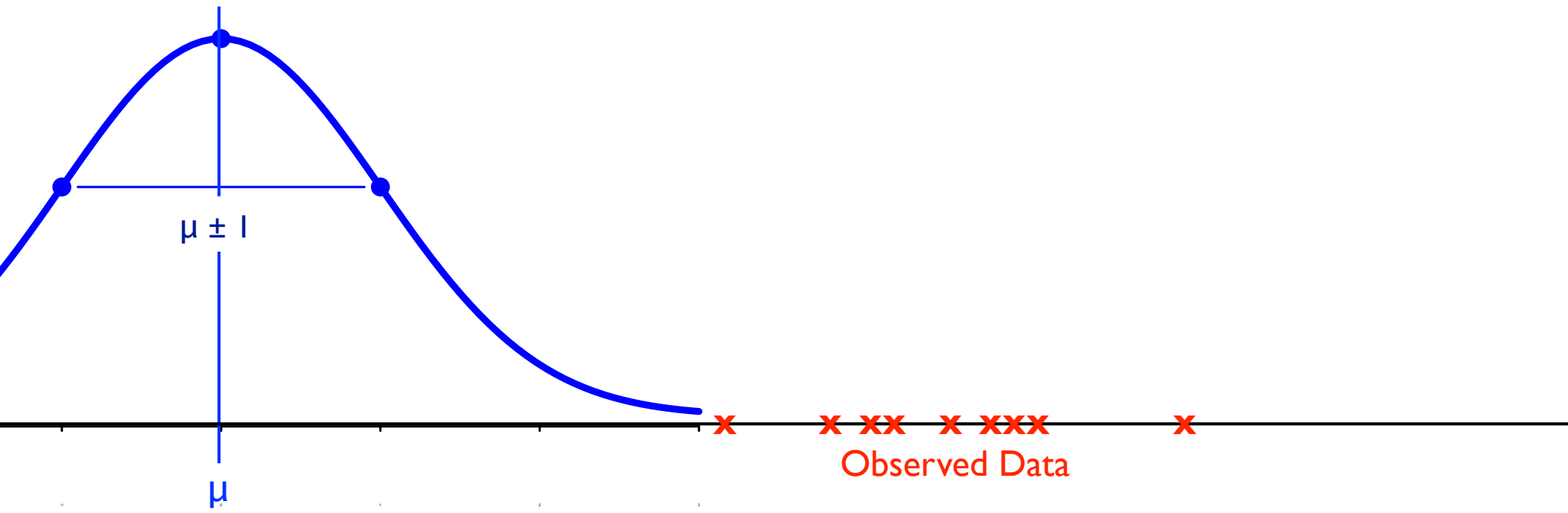


Observed Data

$x \rightarrow$

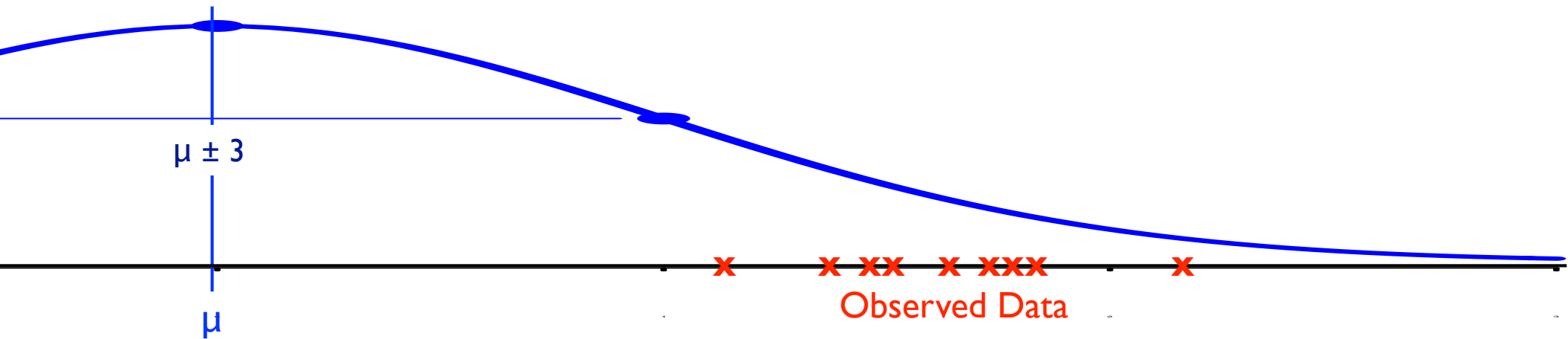
Which is more likely: (a) this?

μ, σ^2 both unknown



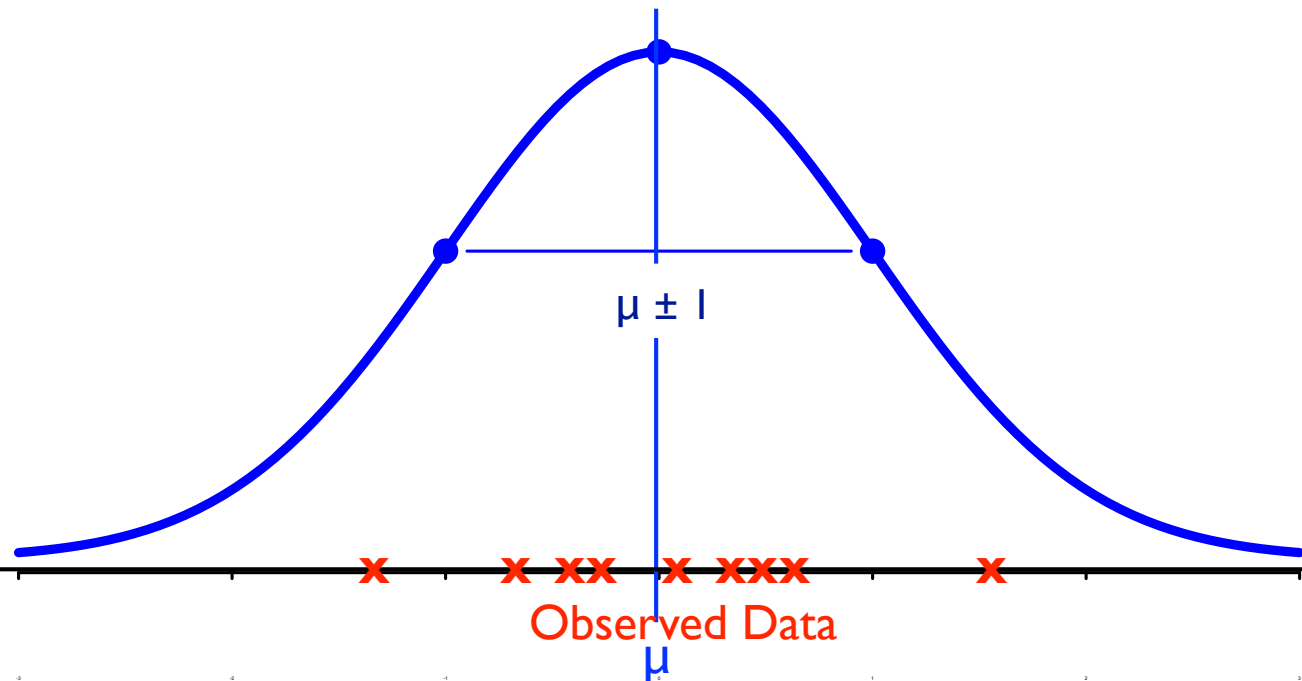
Which is more likely: (b) or this?

μ, σ^2 both unknown



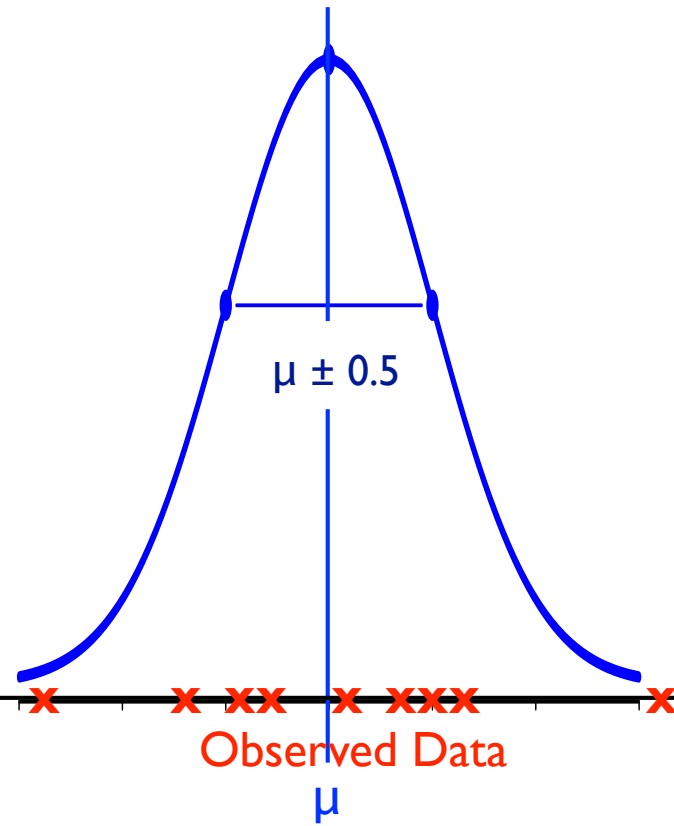
Which is more likely: (c) or this?

μ, σ^2 both unknown



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

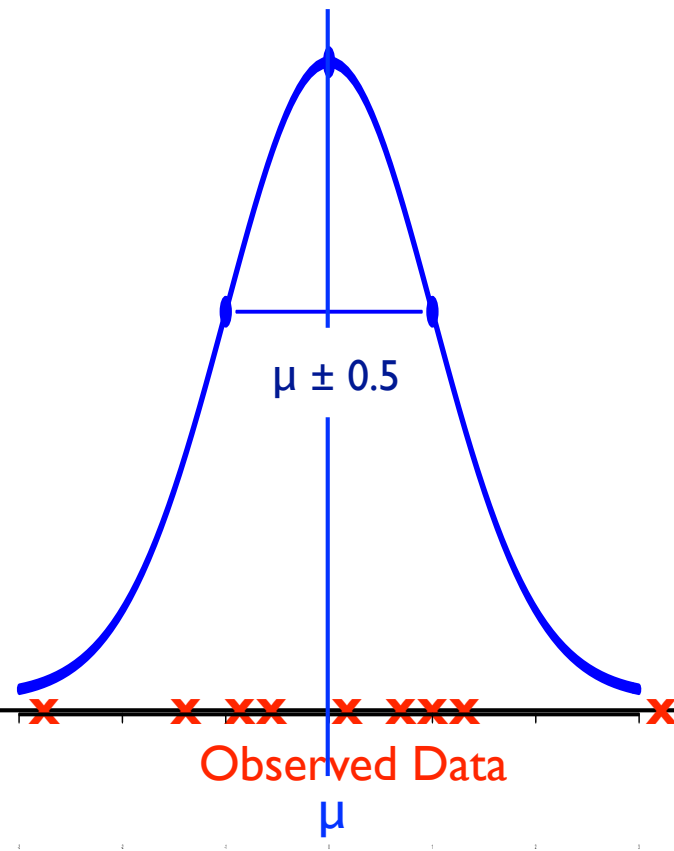
μ, σ^2 both unknown



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 & $\underline{\underline{\sigma^2}}$?



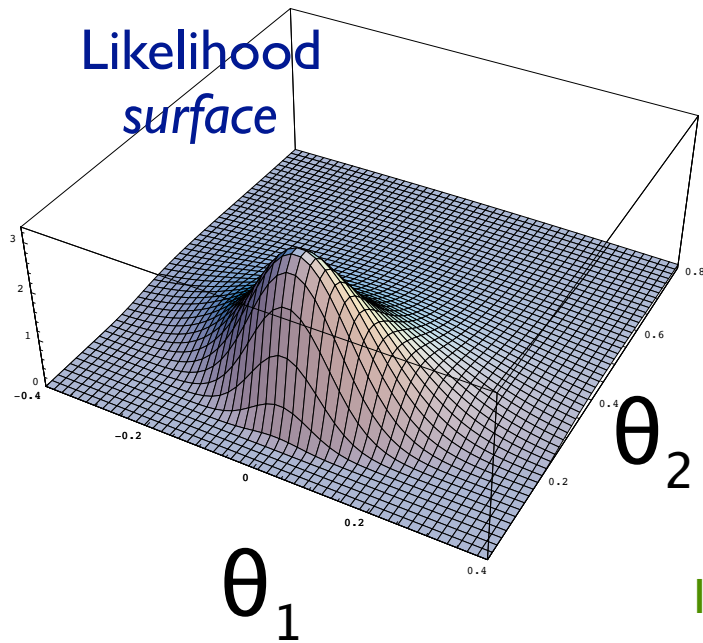
Ex 3: $x_i \sim N(\mu, \sigma^2)$, μ, σ^2 both unknown

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

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

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

Likelihood
surface



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 31

Ex. 3, (cont.)

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

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

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

**Sample variance is MLE of
population variance**

Ex. 3, (cont.)

Defn: An estimator is *unbiased* if expected value = true value

Example: For any distribution, the sample mean $Y = (\sum_{1 \leq i \leq n} X_i)/n$ is an unbiased estimator of population mean since

$$E[Y] = (\sum_{1 \leq i \leq n} E[X_i])/n = n \mu/n = \mu$$

For normal distribution, $(\sum_{1 \leq i \leq n} (X_i - \mu)^2)/n$ is an unbiased est. of σ^2 . Unfortunately, if μ is unknown, estimated *from the same data*, as above, $\hat{\theta}_2 = \sum_{1 \leq i \leq n} \frac{(x_i - \hat{\theta}_1)^2}{n}$ is a consistent, but *biased* estimate of population variance. (An example of *overfitting*.) Unbiased estimate is:

$$\hat{\theta}'_2 = \sum_{1 \leq i \leq n} \frac{(x_i - \hat{\theta}_1)^2}{n-1}$$

i.e., $\lim_{n \rightarrow \infty} =$ correct

Moral: MLE is a great idea, but not a magic bullet

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 pmf or pdf of the model) is often the critical step; the math/algorithms to optimize it are generic

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

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*

Conditional Probability & Bayes Rule

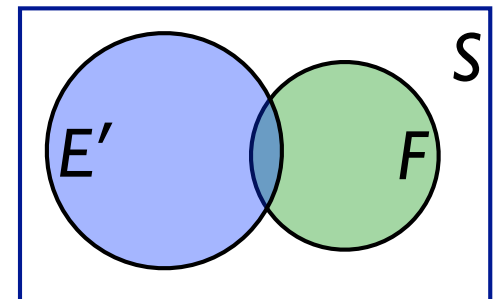
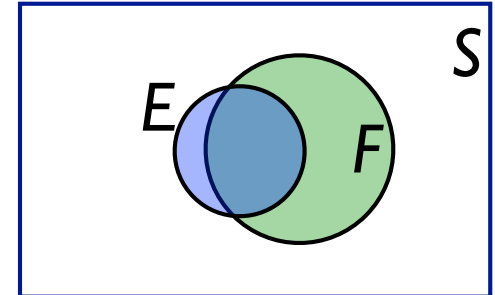
conditional probability

Conditional probability of E given F: probability that E occurs given that F has occurred.

“Conditioning on F”

Written as $P(E|F)$

Means “P(E has happened, given F observed)”

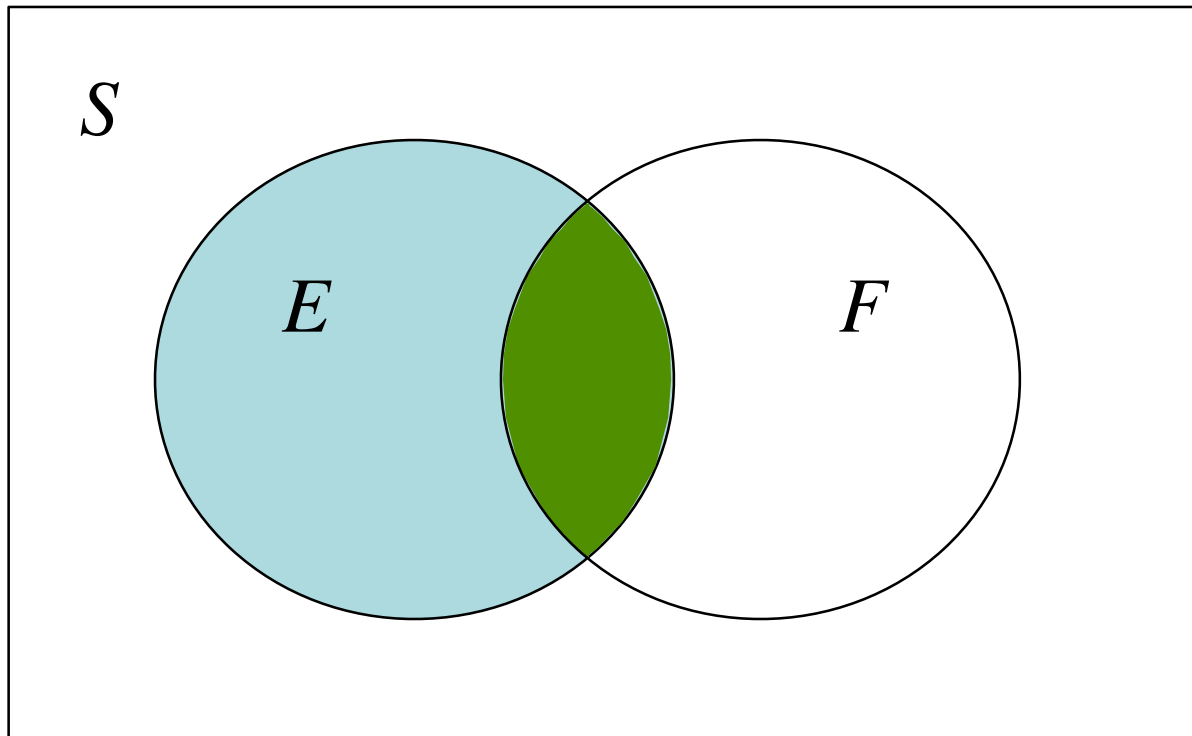


$$P(E | F) = \frac{P(EF)}{P(F)}$$

where $P(F) > 0$

E and F are events in the sample space S

$$E = EF \cup EF^c$$



$$EF \cap EF^c = \emptyset$$

$$\Rightarrow P(E) = P(EF) + P(EF^c)$$

Most common form:

$$P(F | E) = \frac{P(E | F)P(F)}{P(E)}$$

Expanded form (using law of total probability):

$$P(F | E) = \frac{P(E | F)P(F)}{P(E | F)P(F) + P(E | F^c)P(F^c)}$$

Proof:

$$P(F | E) = \frac{P(EF)}{P(E)} = \frac{P(E | F)P(F)}{P(E)}$$

EM

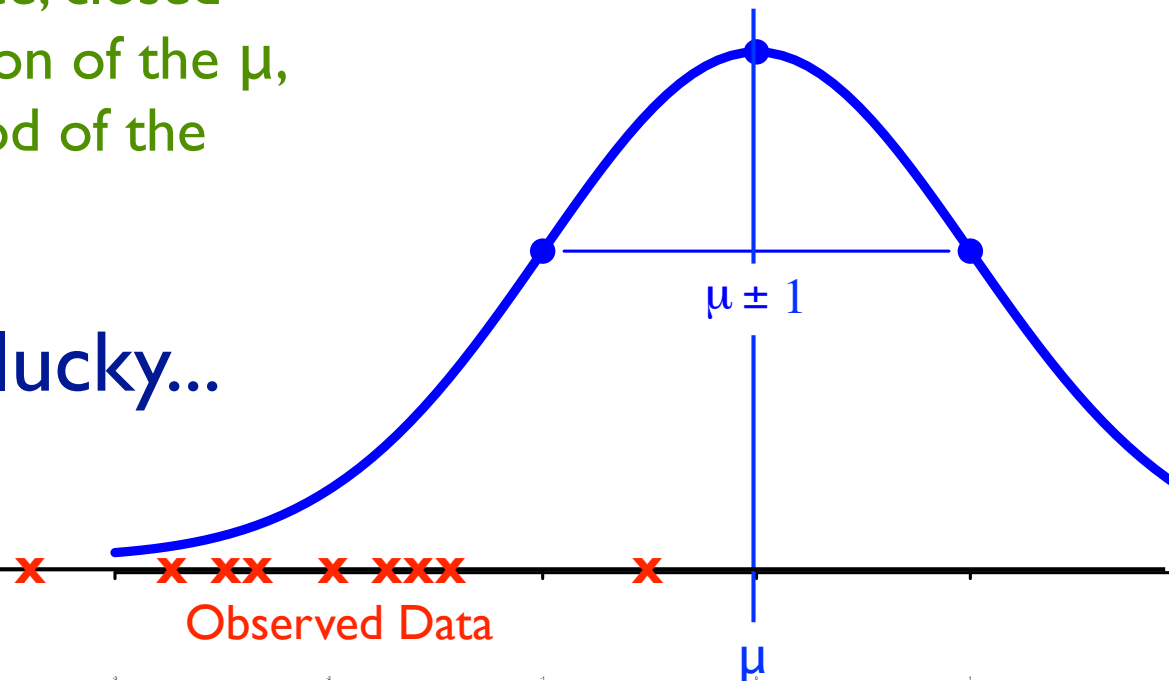
The Expectation-Maximization Algorithm
(for a Two-Component Gaussian Mixture)

Previously:

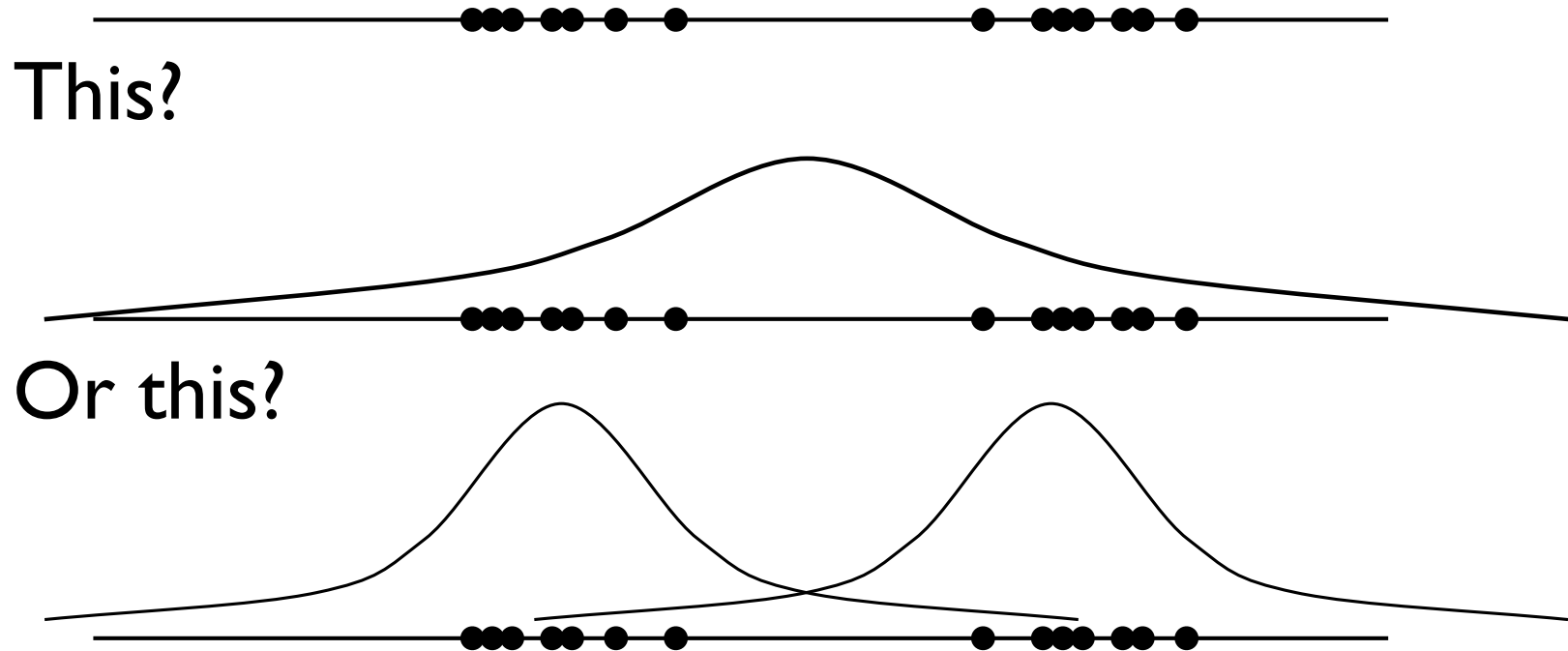
How to estimate μ given data

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...

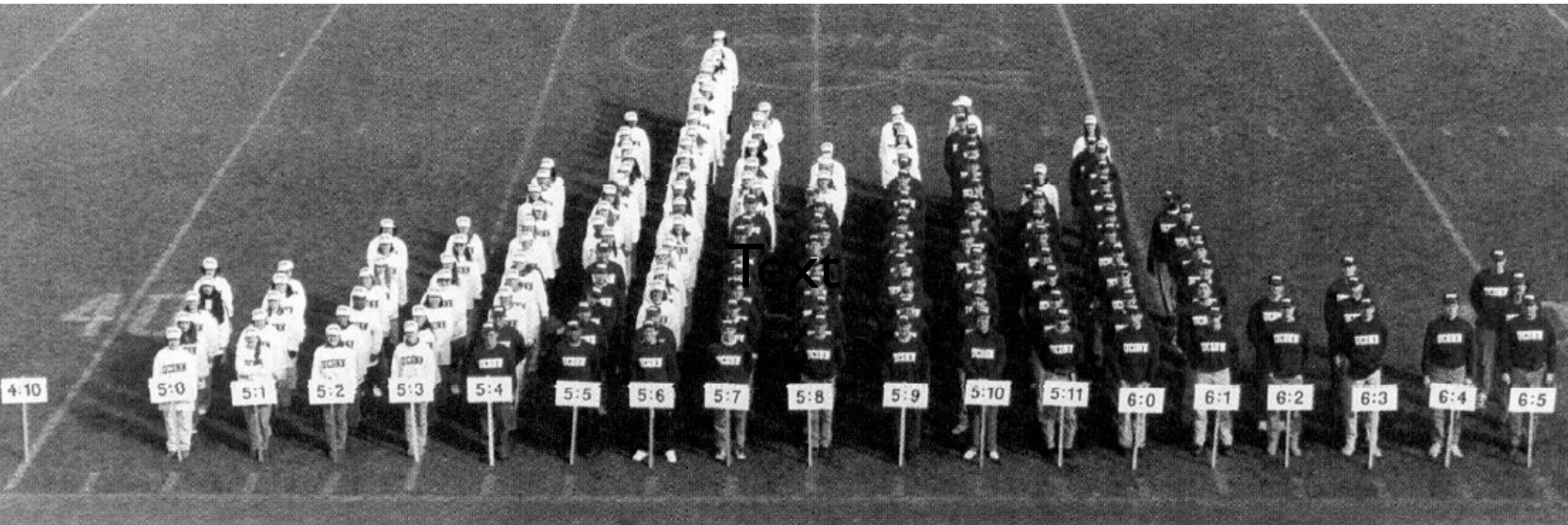


More Complex Example



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

A Living Histogram

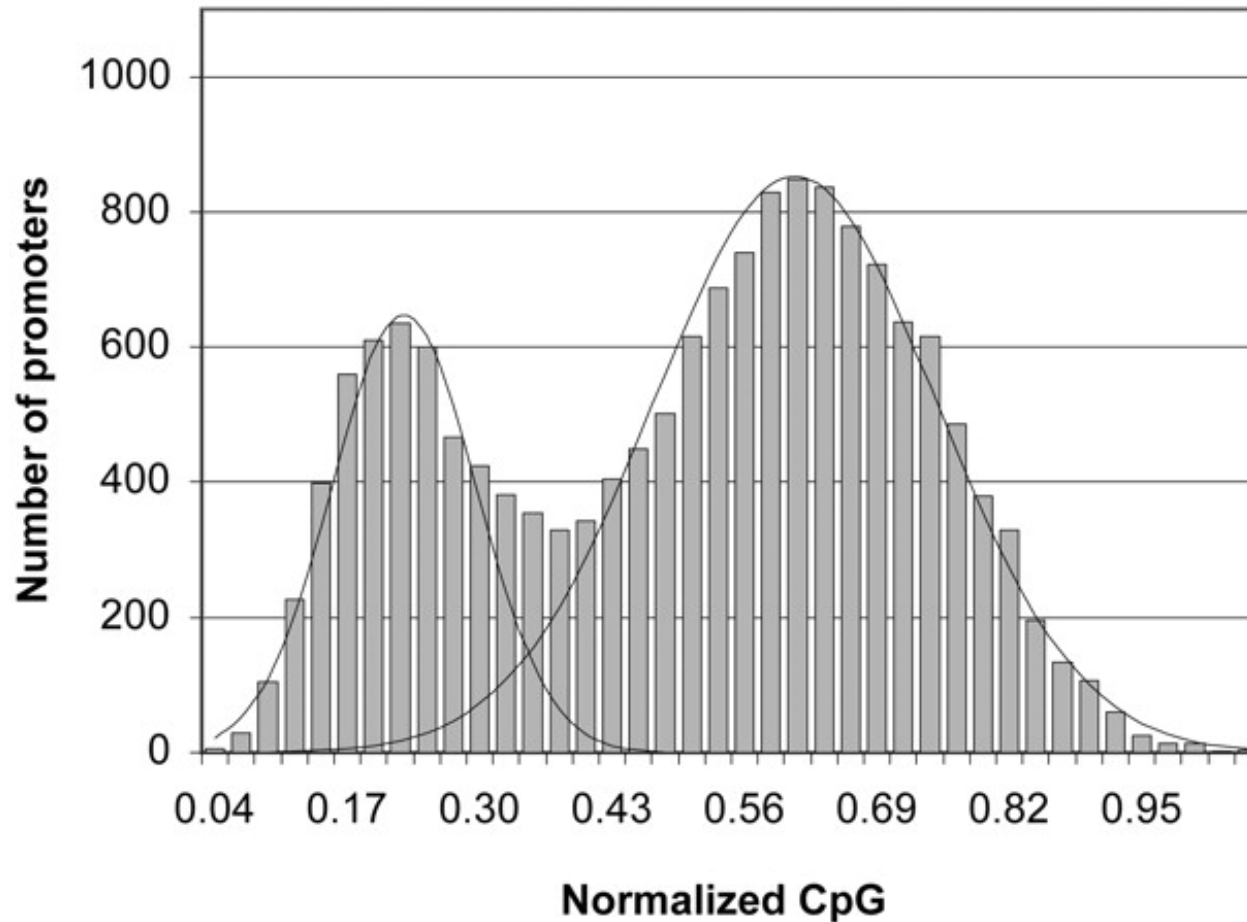


male and female genetics students, University of Connecticut in 1996

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

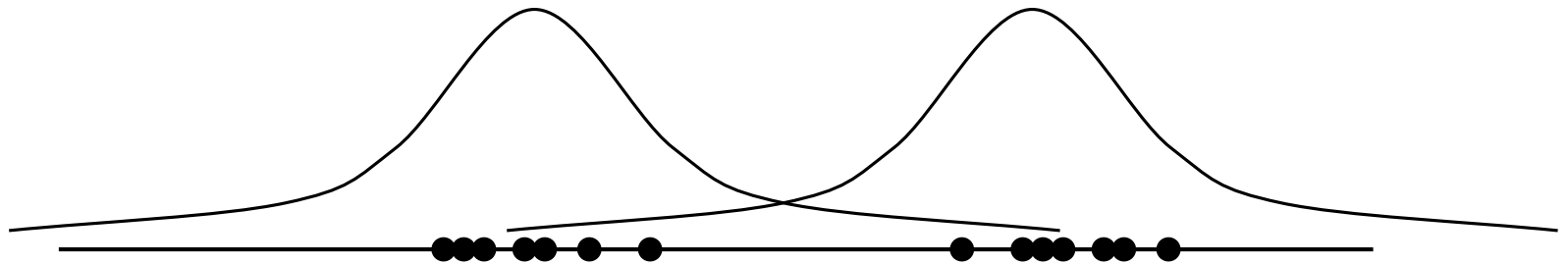
Another Real Example:

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	$\tau_2 = 1 - \tau_1$

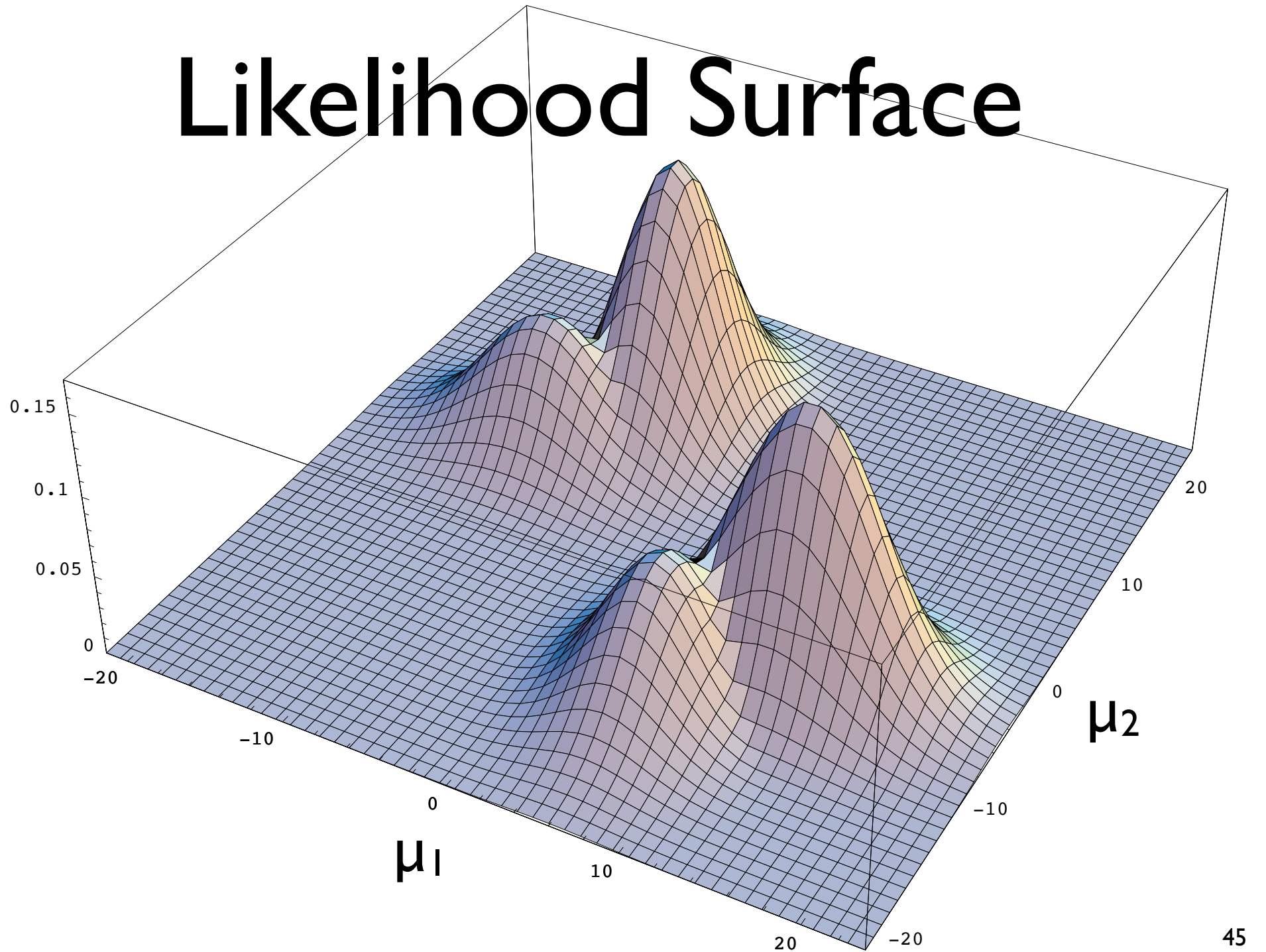
P.D.F. $\xrightarrow{\text{separately}}$ $f(x|\mu_1, \sigma_1^2)$ $f(x|\mu_2, \sigma_2^2)$

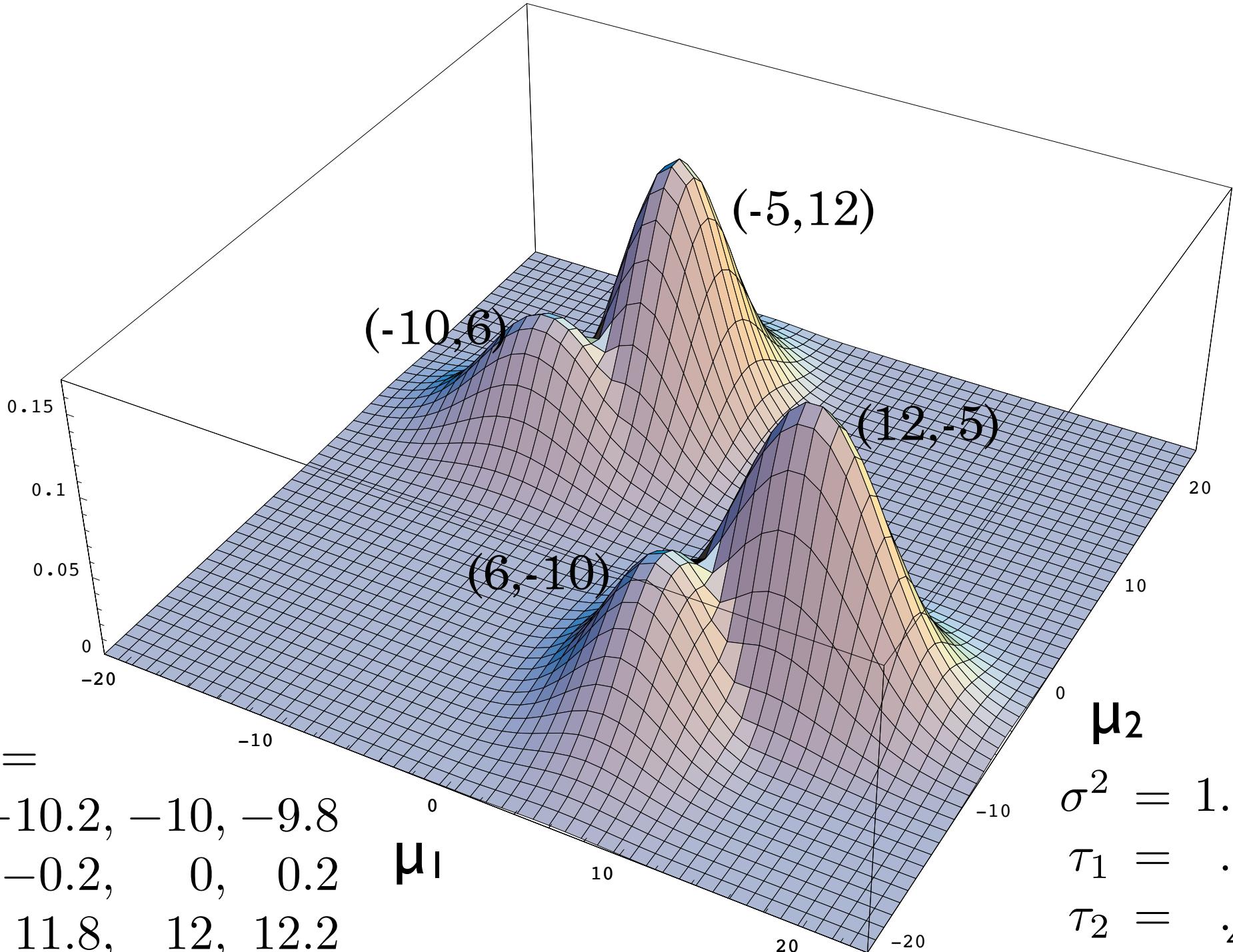
$\xrightarrow{\text{together}}$ $\tau_1 f(x|\mu_1, \sigma_1^2) + \tau_2 f(x|\mu_2, \sigma_2^2)$

Likelihood $\left\{ \begin{aligned} &L(x_1, x_2, \dots, x_n | \mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \tau_1, \tau_2) \\ &= \prod_{i=1}^n \sum_{j=1}^2 \tau_j f(x_i | \mu_j, \sigma_j^2) \end{aligned} \right.$

No closed-form max

Likelihood Surface





$x_i =$
 $-10.2, -10, -9.8$
 $-0.2, 0, 0.2$
 $11.8, 12, 12.2$

μ_1

μ_2
 $\sigma^2 = 1.0$
 $\tau_1 = .5$
 $\tau_2 = .5$

A What-If Puzzle

Likelihood

$$L(x_1, x_2, \dots, x_n | \overbrace{\mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \tau_1, \tau_2}^{\theta})$$
$$= \prod_{i=1}^n \sum_{j=1}^2 \tau_j f(x_i | \mu_j, \sigma_j^2)$$

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

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

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

A Hat Trick

Two slips of paper in a hat:

Pink: $\mu = 3$, and

Blue: $\mu = 7$.

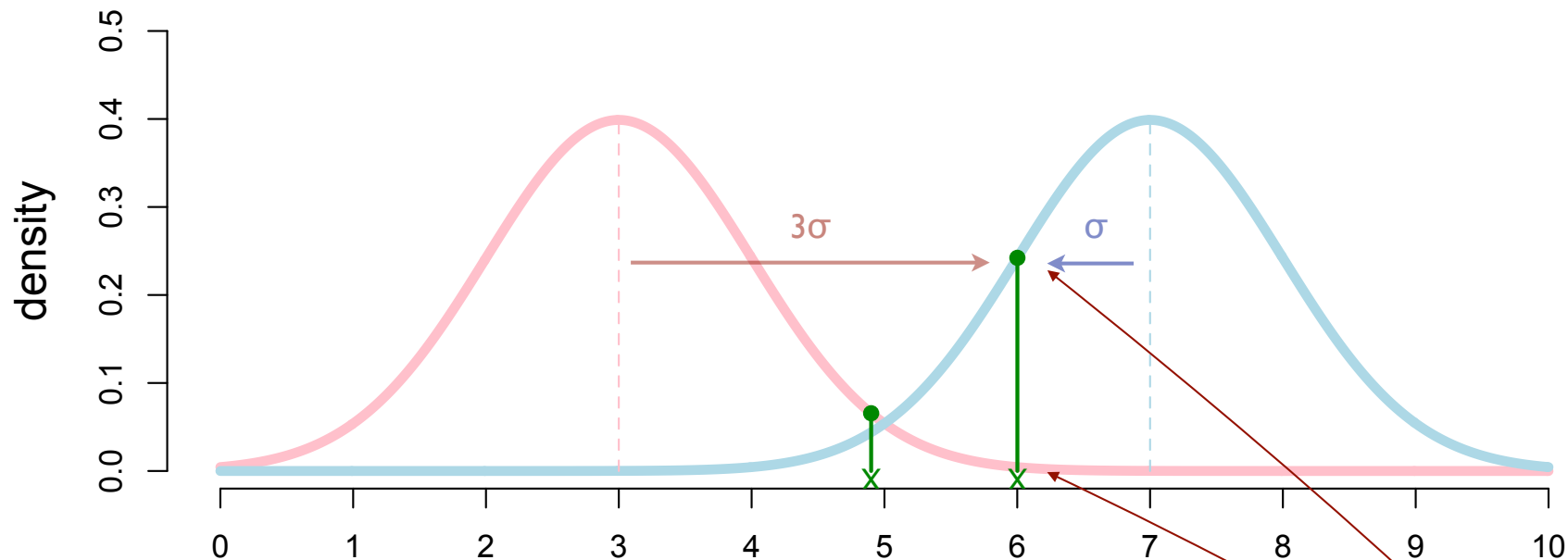
You draw one, then (without revealing color or μ) reveal a single sample $X \sim \text{Normal}(\text{mean } \mu, \sigma^2 = 1)$.

You happen to draw $X = 6.001$.

Dr. Mean says “your slip = 7.” What is $P(\text{correct})$?

What if X had been 4.9?

A Hat Trick



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

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

$$P(\mu = 7|X \approx 6) = \frac{P(X \approx 6|\mu = 7)P(\mu = 7)}{P(X \approx 6)} \quad \text{Bayes rule}$$

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

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

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

f = normal density

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

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

$E[Y] = \mu$

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

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

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

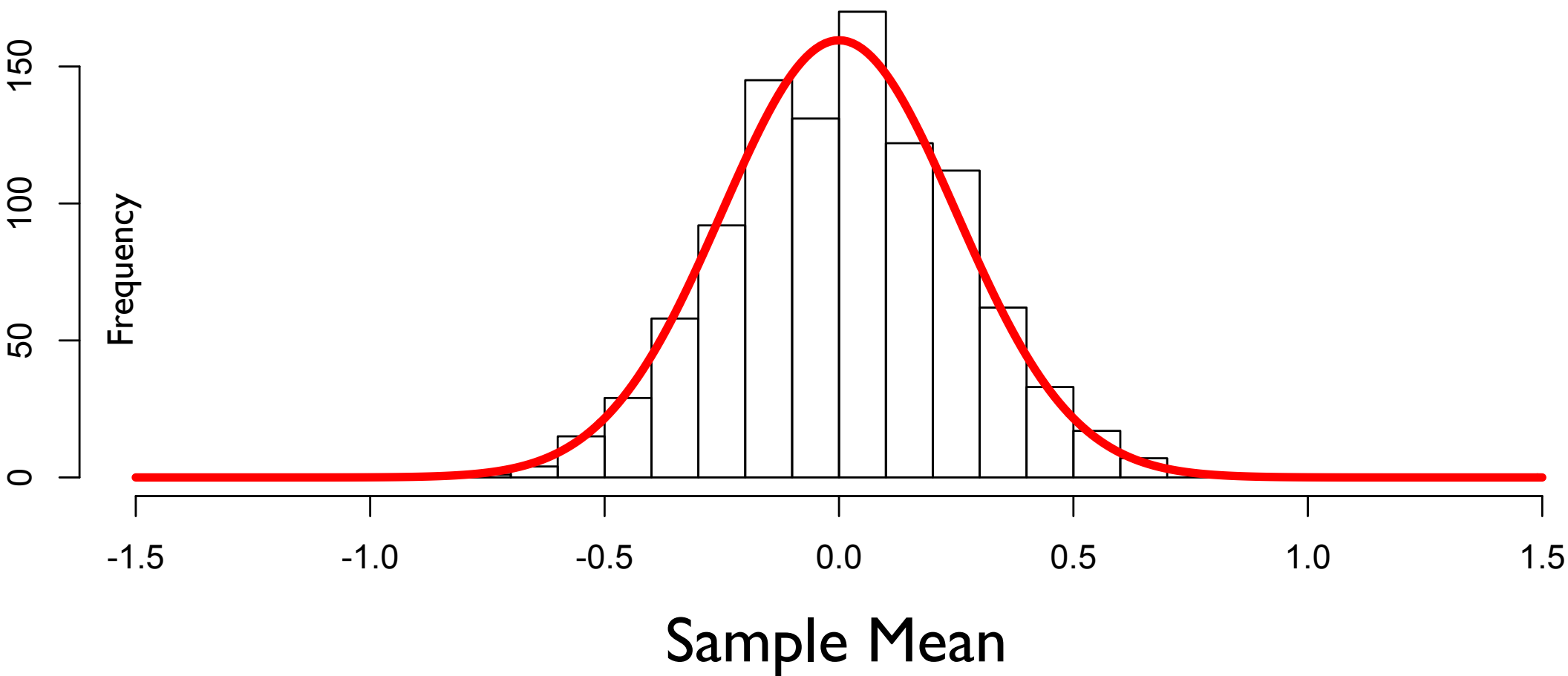
“ Y within ± 0.5 of μ ” = “ Y within $\pm 2 \sigma$ of μ ” $\approx 95\%$ prob

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, perhaps)

Histogram of 1000 samples of the average of 16 $N(0,1)$ RVs
Red = $N(0, 1/16)$ density

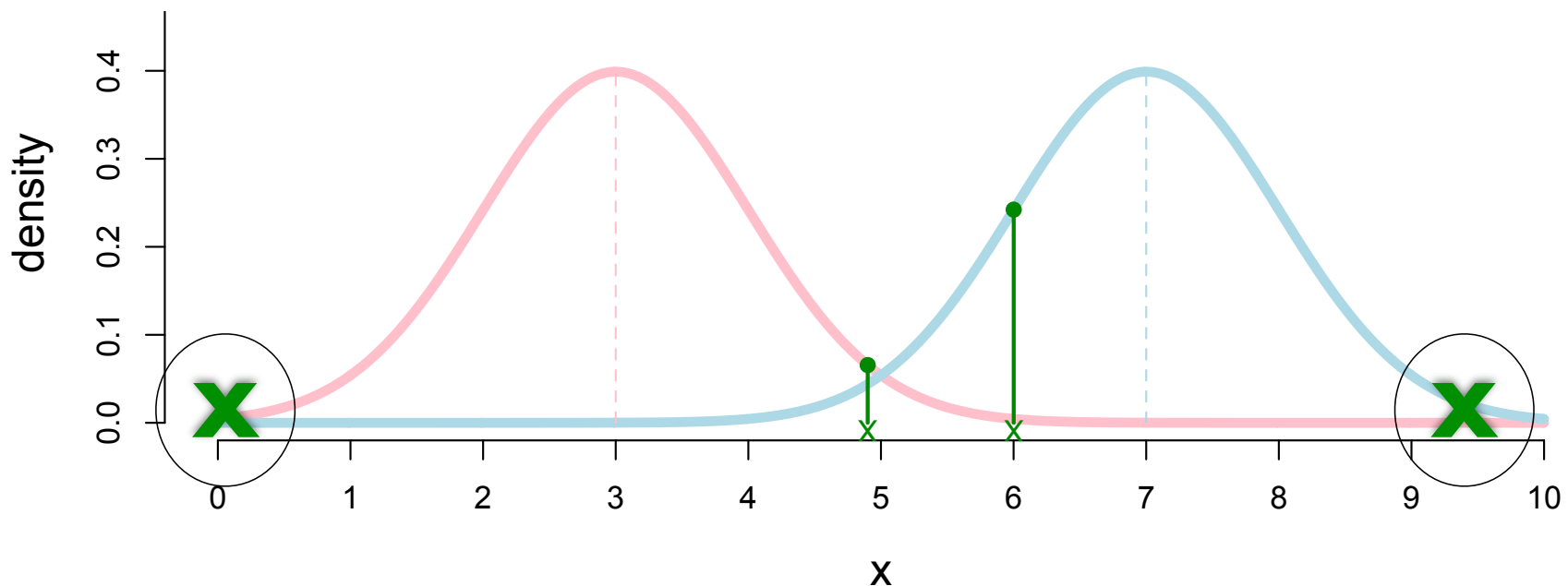


Hat Trick 2 (cont.)

Note 2 (Important):

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



A What-If Puzzle

Likelihood

$$L(x_1, x_2, \dots, x_n \mid \overbrace{\mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \tau_1, \tau_2}^{\theta})$$
$$= \prod_{i=1}^n \sum_{j=1}^2 \tau_j f(x_i \mid \mu_j, \sigma_j^2)$$

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

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

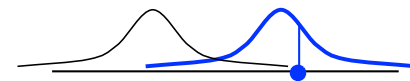
$$z_{ij} = \begin{cases} 1 & \text{if } x_i \text{ drawn from } f_j \\ 0 & \text{otherwise} \end{cases}$$

EM as Egg vs Chicken

Hat
Trick 1

IF parameters θ known, could estimate z_{ij}

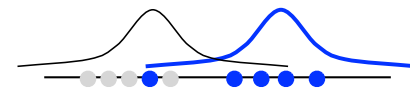
E.g., $|x_i - \mu_1|/\sigma_1 \gg |x_i - \mu_2|/\sigma_2 \Rightarrow P[z_{i1}=1] \ll P[z_{i2}=1]$



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

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

Simple Version: “Classification EM”

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.

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

“K-means clustering,”
essentially

Full EM

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

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

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

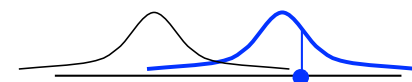
$$L(x_1, \dots, x_n, z_{11}, z_{12}, \dots, z_{n2} \mid \theta) \quad \text{(complete data likelihood)}$$

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

Instead, maximize *expected* likelihood of visible data

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

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 $P(A|D)$

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

$$E[z_{i1}] = P(A|D) = \frac{P(D|A)P(A)}{P(D)}$$

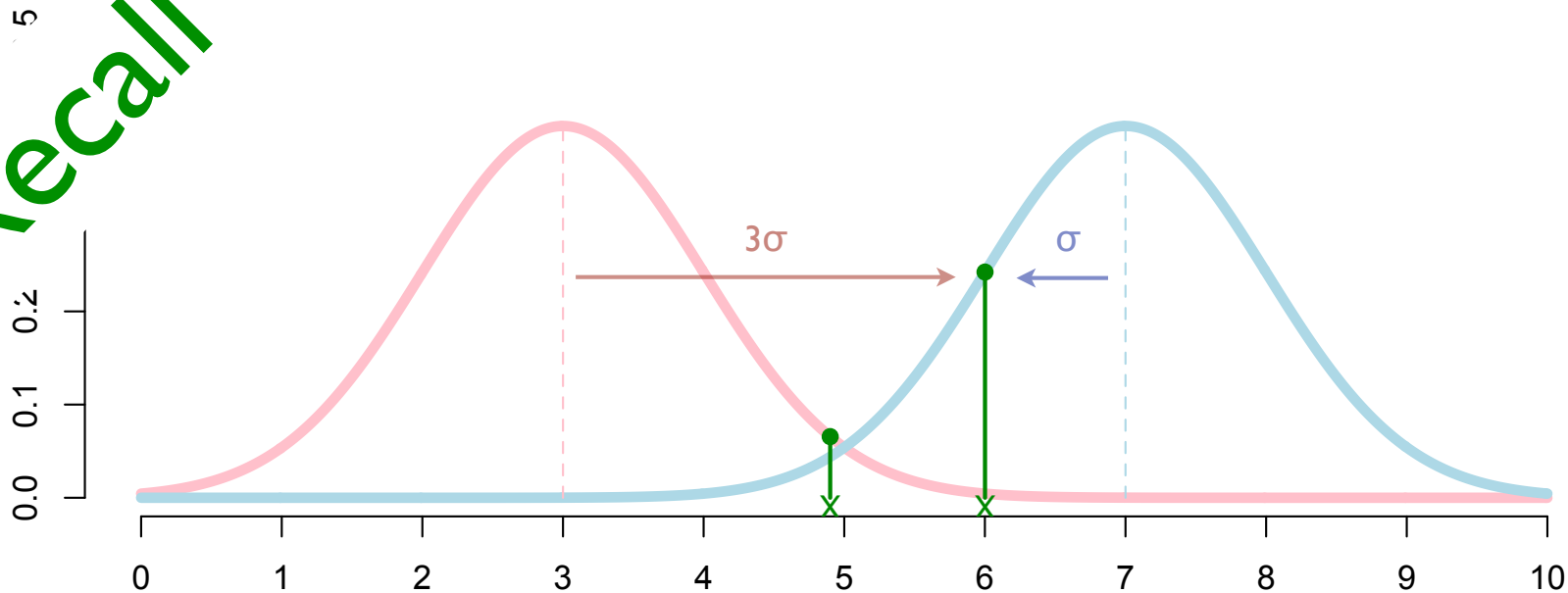
$$\begin{aligned} P(D) &= P(D|A)P(A) + P(D|B)P(B) \\ &= f_1(x_i|\theta_1)\tau_1 + f_2(x_i|\theta_2)\tau_2 \end{aligned}$$

Repeat for each $z_{i,j}$

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

A Hat Trick

der Recall



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

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

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

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

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

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

$E[Z_{i,\text{pink}}] = ?$

$E[Z_{i,\text{blue}}] = ?$

$f = \text{normal density}$

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,

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

equal, if z_{ij} are 0/1



Formulas with “if’s” are messy; can we blend more smoothly?

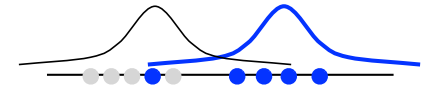
Yes, many possibilities. Idea 1:

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

Idea 2 (Better):

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

M-step:



Find θ maximizing $E(\log(\text{Likelihood}))$

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

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

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

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:

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

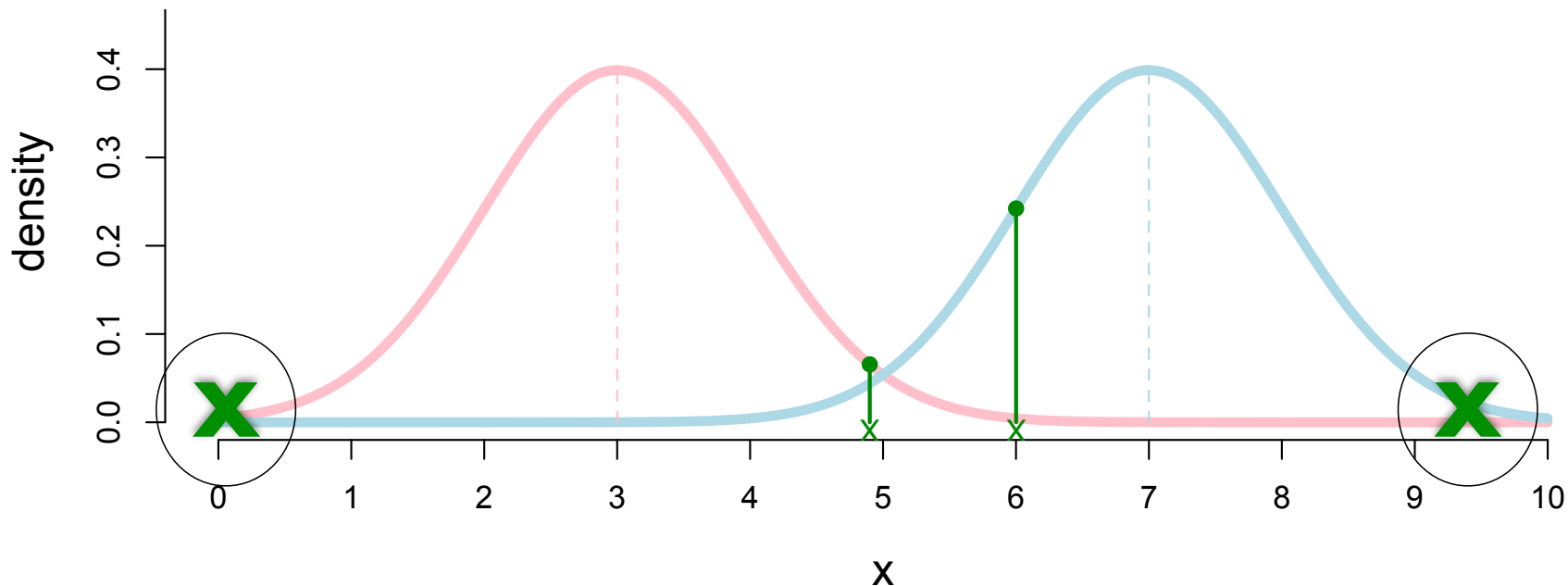
Recall

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	31.02	10.66
E[z _{i2}]x _i	0.1	0.2	3.3	15.2	19.4	20.8	58.98	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 $E[\log \text{likelihood}]$

given $E[z]$ [where “ $E[\log L]$ ” is wrt random $z \sim E[z] = p(z=1)$]

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, ...

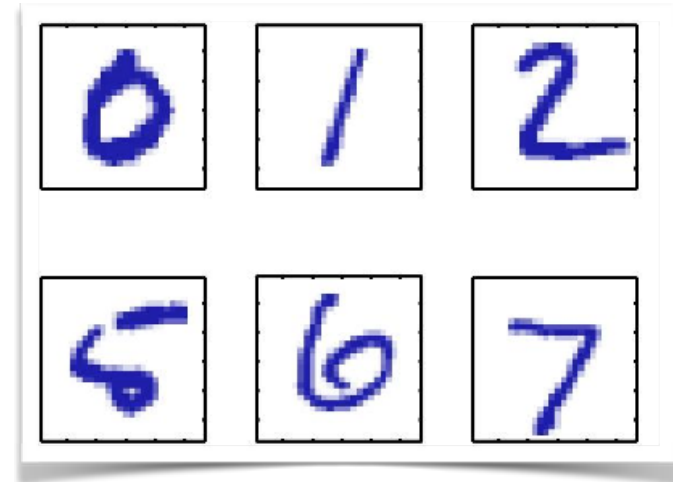
A “Machine Learning” Example

Handwritten Digit Recognition

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

A Bio Example

A time series:

Feel good; catch flu; sick as dog; meh; OK again

Measure gene expression at each point

Hypothesis: genes that co-vary are co-involved

Possible approach: do the genes fall into a few “clusters,” say, as defined by Gaussian distributions (in high dimension, not one-D)

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:

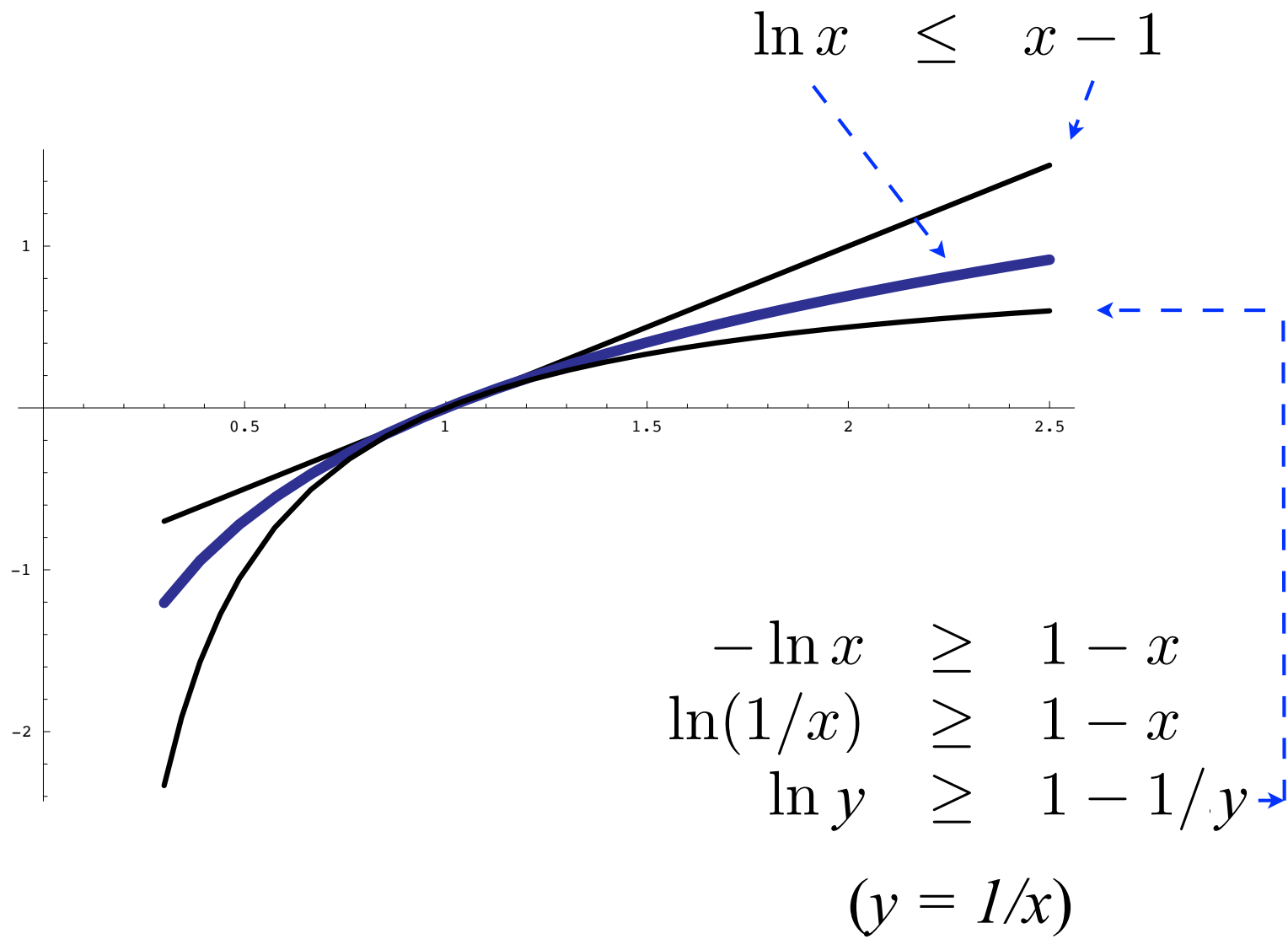
Let $P(x) \log \frac{P(x)}{Q(x)} = 0$ if $P(x) = 0$ [since $\lim_{y \rightarrow 0} y \log y = 0$]

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?



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 $P \neq Q$, then

$P(x) > Q(x) \Rightarrow \log(P(x)/Q(x)) > 0$

and

$P(y) < Q(y) \Rightarrow \log(P(y)/Q(y)) < 0$

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”