CSE 427

Winter 2021

MLE, EM

Outline

HW#1 Discussion

MLE: Maximum Likelihood Estimators

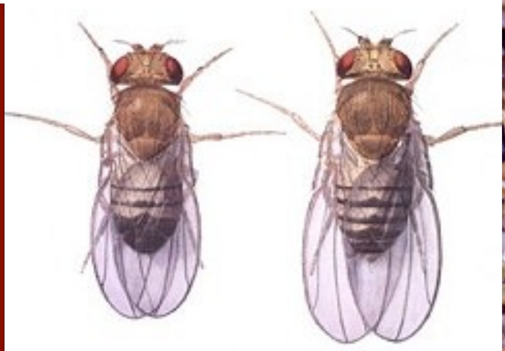
EM: the Expectation Maximization Algorithm

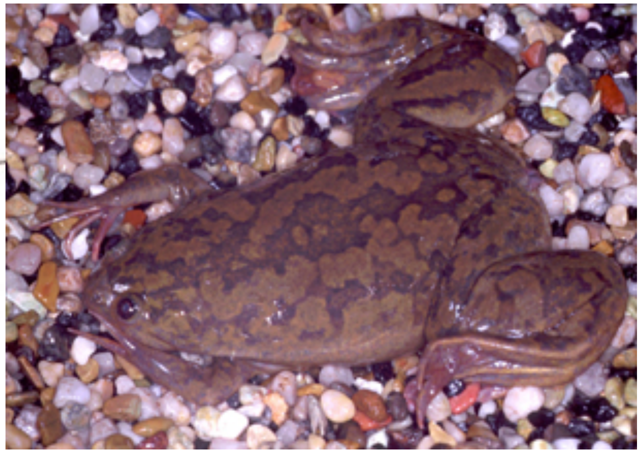
Next: Motif description & discovery

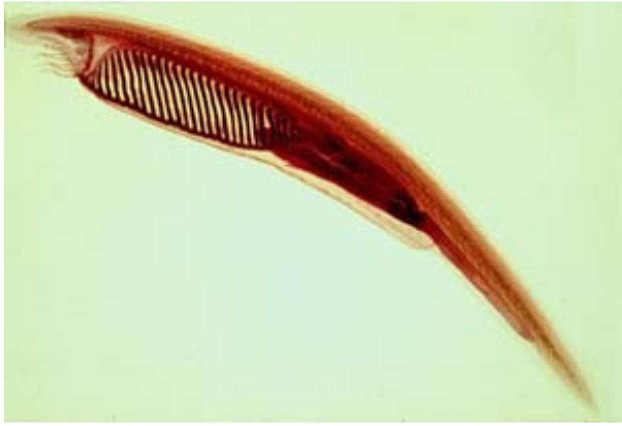
HW # 1 Discussion

	Species	Name	Description	Access-ion	score to #1
1	Homo sapiens (Human)	MYOD1_HUMAN	Myoblast determination protein 1	P15172	1709
2	Homo sapiens (Human)	TAL1_HUMAN	T-cell acute lymphocytic leukemia protein 1 (TAL-1)	P17542	143
3	Mus musculus (Mouse)	MYOD1_MOUSE	Myoblast determination protein 1	P10085	1500
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


Courtesy of Ralf Sommer

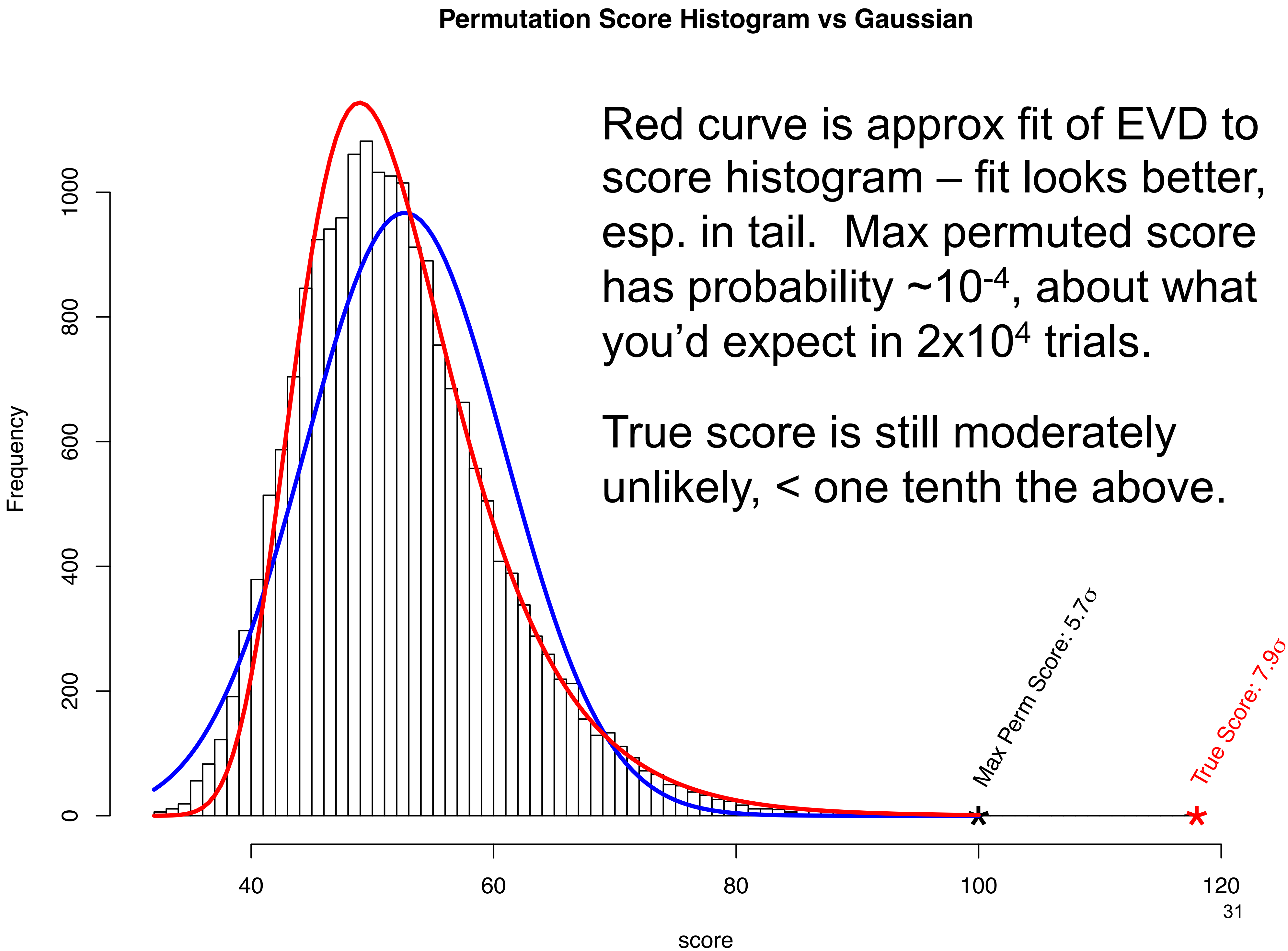






MyoD

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



Red curve is approx fit of EVD to score histogram – fit looks better, esp. in tail. Max permuted score has probability ~10^{-4}, about what you'd expect in 2×10^4 trials.

True score is still moderately unlikely, < one tenth the above.

Full pairwise score table, reordered

```
## ...... hsMYOD mmMYOD ggMYOD xlMYOD drMYOD bbQ8IU dmMYOD hsTAL1 eLIN32 hsSYFM
```

```
##        P15172 P10085 P16075 P13904 Q90477 Q8IU24 P22816 P17542 Q10574 O95363
## P15172   1709   1500   1020    978    893    428    368    143    118     56
## P10085   1500   1702   1043   1002    925    440    367    128    118     52
## P16075   1020   1043   1594   1147   1093    448    414    129    120     61
## P13904    978   1002   1147   1541   1104    450    410    128    120     72
## Q90477    893    925   1093   1104   1479    449    410    112    117     62
## Q8IU24    428    440    448    450    449   1215    446    144    125     45
## P22816    368    367    414    410    410    446   1746    123    124     74
## P17542    143    128    129    128    112    144    123   1731    156     66
## Q10574    118    118    120    120    117    125    124    156    746     67
## O95363     56     52     61     72     62     45     74     66     67   2420
```

`species - hs,mm, gg=chick, cl=frog, bb=amphioxus, fly, elegans`

Learning From Data: MLE

Maximum Likelihood Estimators

Parameter Estimation

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

Not formally "conditional probability," but the notation is convenient…

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

(For *Discrete* Distributions)

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

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

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

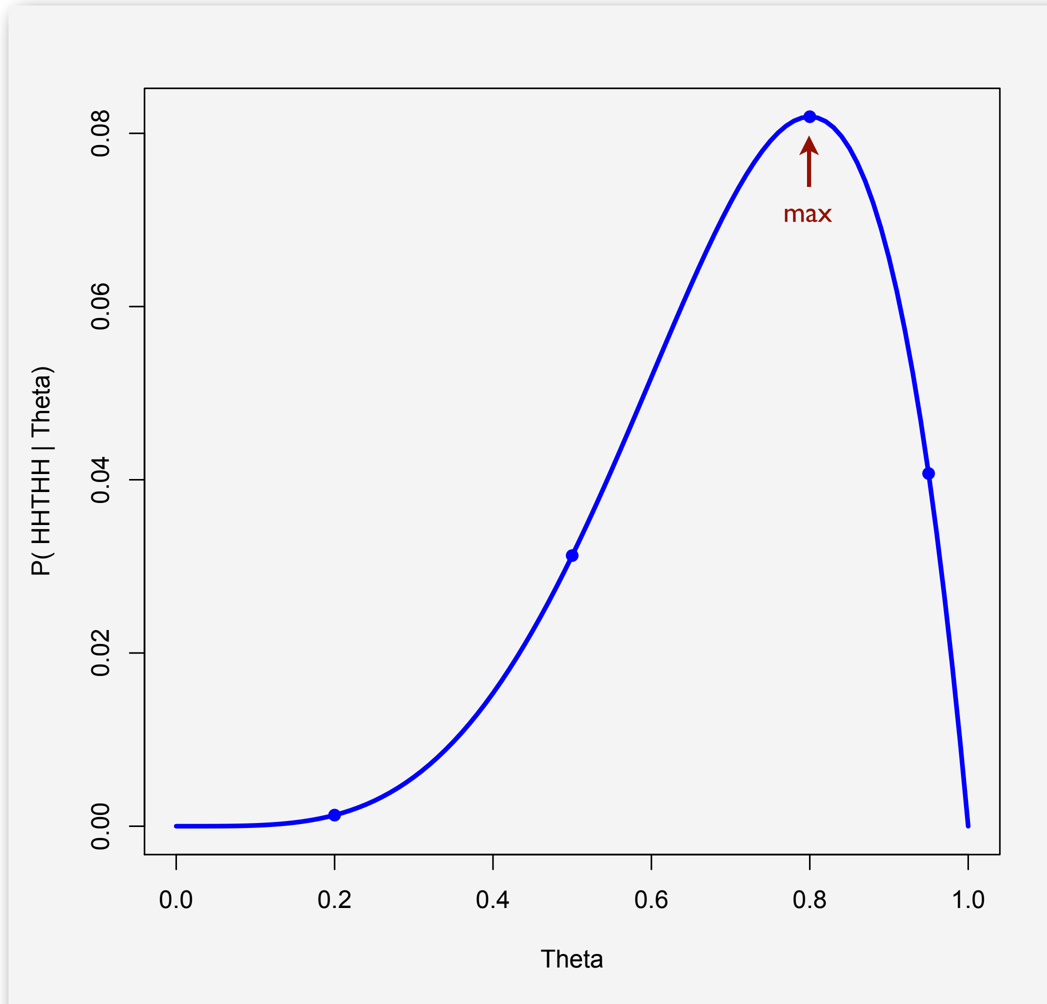
Viewed as a function of θ (fixed x), it's called *likelihood*

- E.g., $\Sigma_\theta P(x \mid \theta)$ can be anything; *relative* values are the focus.
- 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

(For *Discrete* Distributions)

One (of many) approaches to param. est.

Likelihood of (indp) observations $x_1, x_2, \ldots, x_n$

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

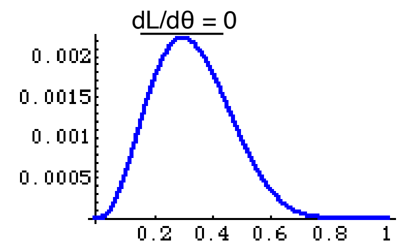
As a function of θ, *what θ maximizes the likelihood of the data actually observed?*

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 1

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



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

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)

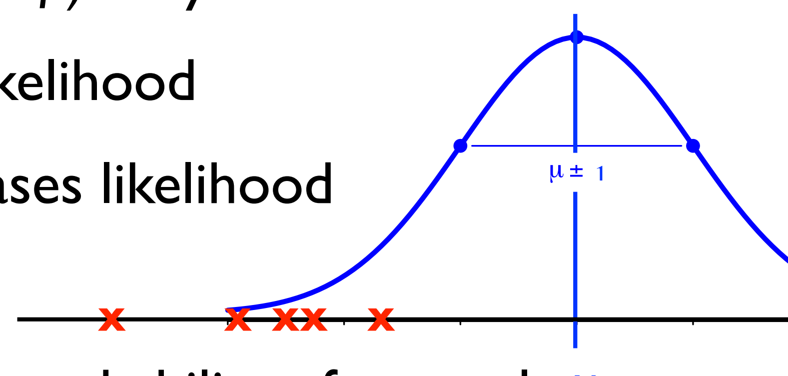
Likelihood

(For *Continuous* Distributions)

Pr(any specific x_i) = *0,* so "likelihood = probability" won't work. D<u>efn:</u> "likelihood" of $x_1, \ldots, x_n$ is their *joint density;* = (by indp) 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 δ>0, the probability of a sample within ±δ/2 of x is ≈ δ$f(x)$, so density really *is* capturing probability, and δ is *constant* wrt θ, so it just drops out of d/dθ log $L(\ldots)$ = 0.

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

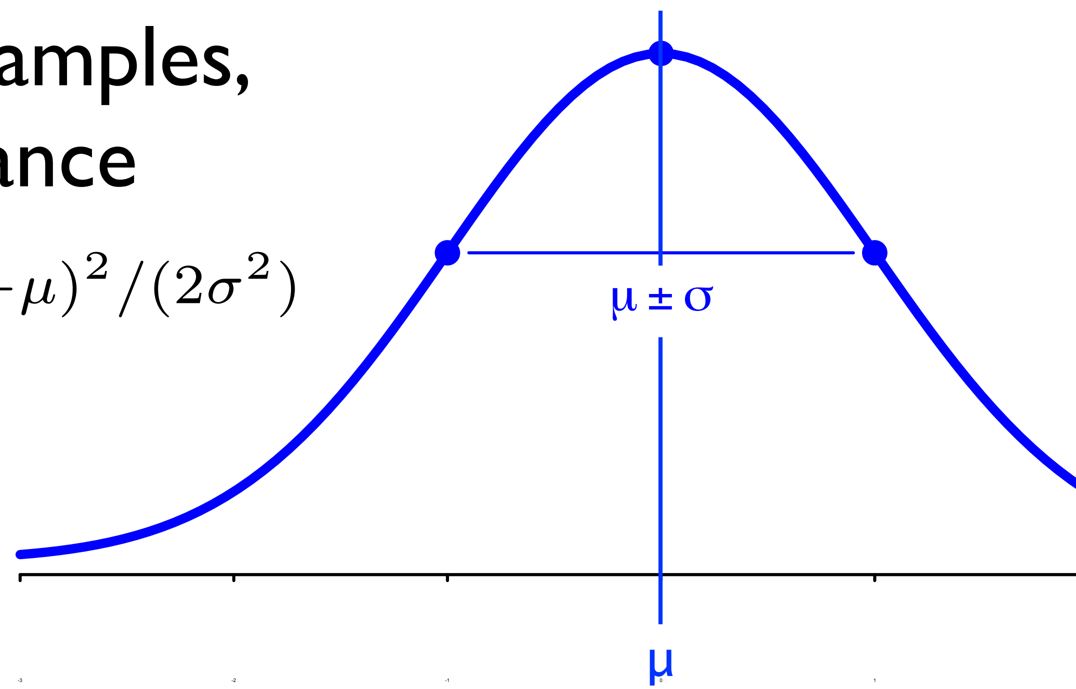
Parameter Estimation

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

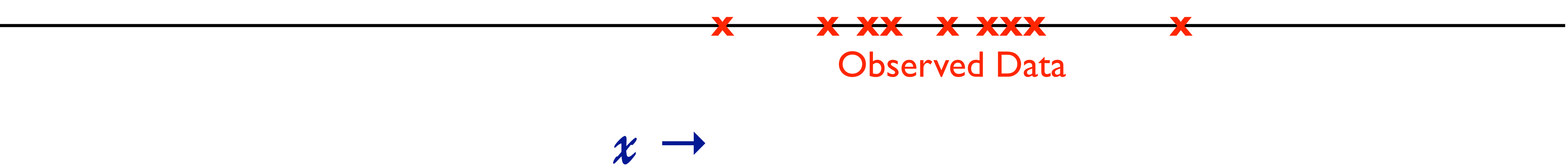
E.g.: Given *n normal* samples, estimate mean & variance

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

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

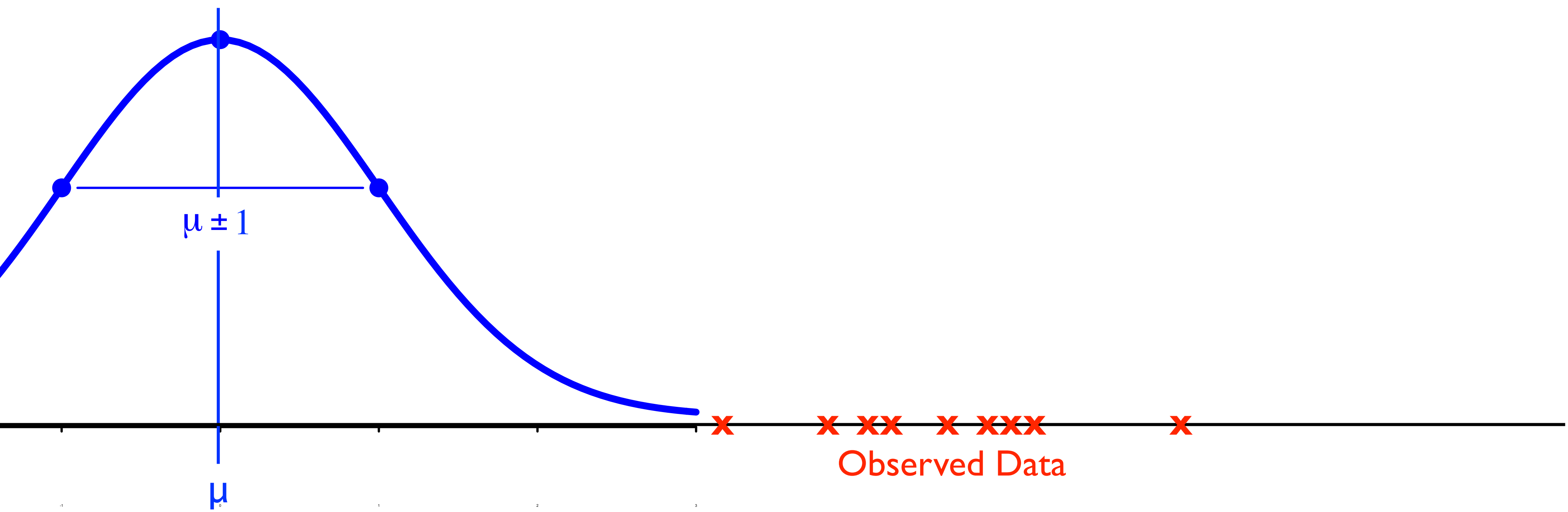


Ex2: I got data; a little birdie tells me it's normal, and promises $\sigma^2 = 1$



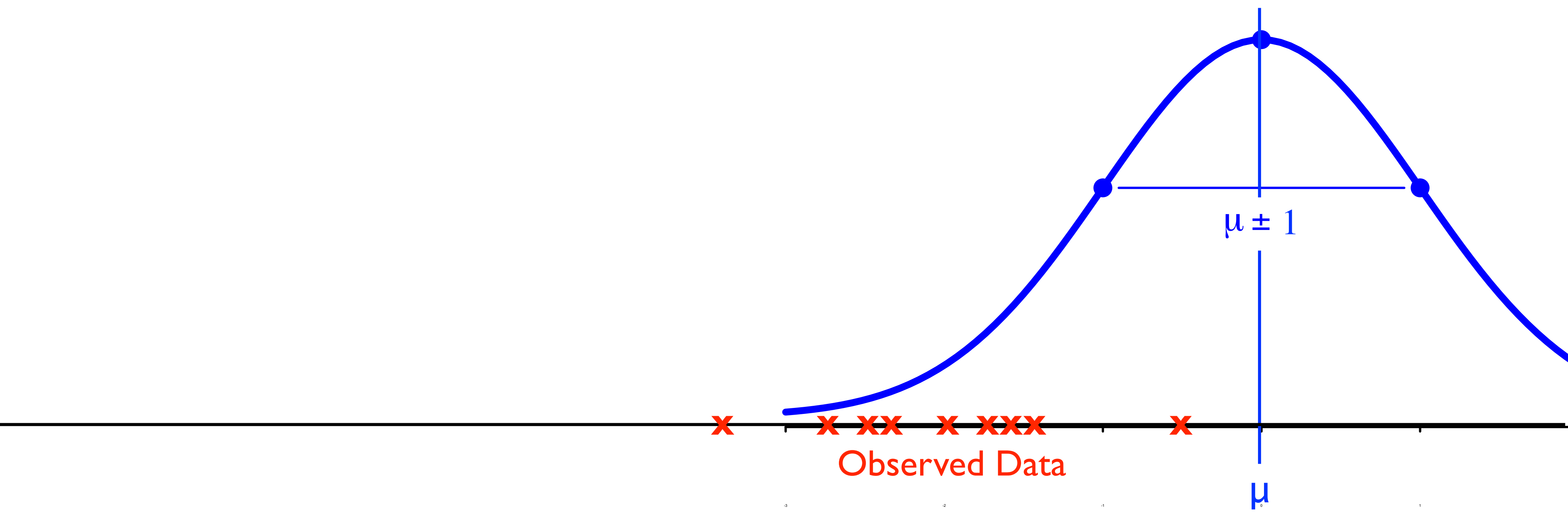
Which is more likely: (a) this?

μ unknown, $\sigma^2 = 1$



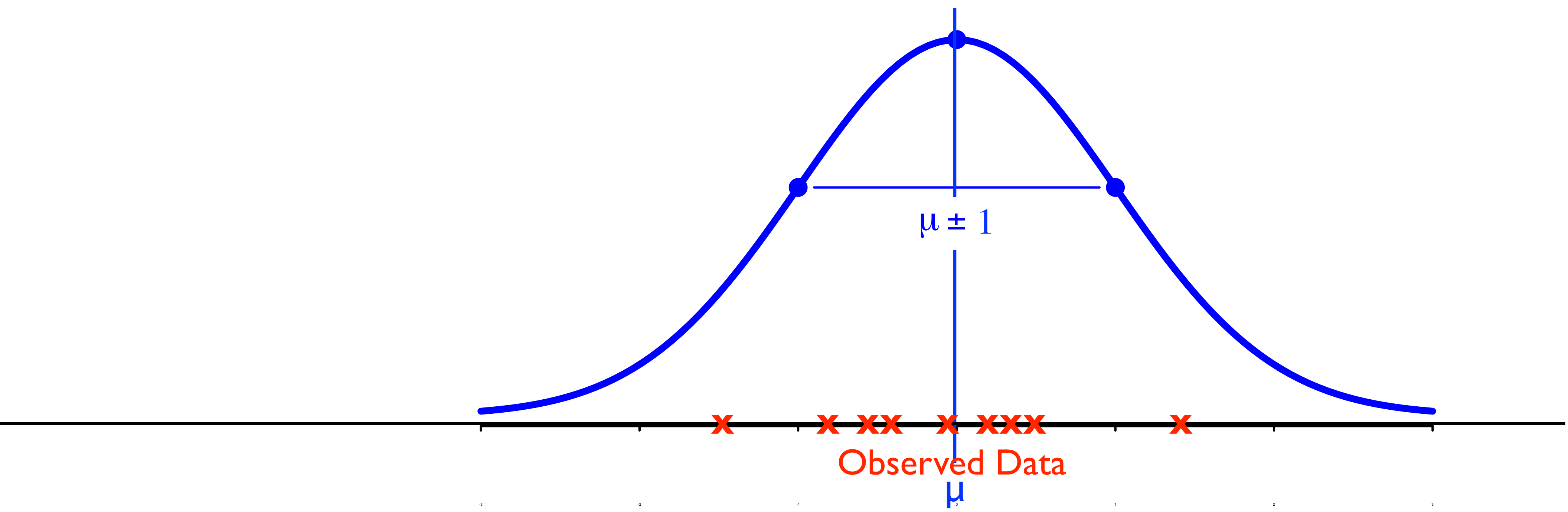
Which is more likely: (b) or this?

μ unknown, $\sigma^2 = 1$



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

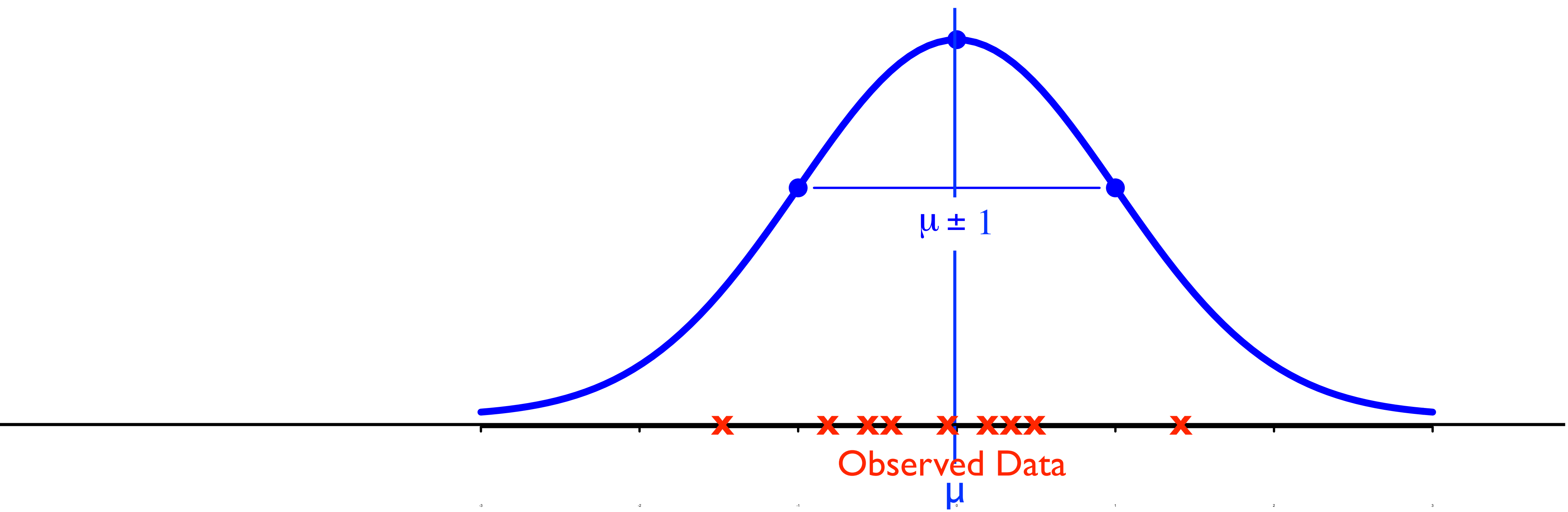
μ unknown, $\sigma^2 = 1$



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

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

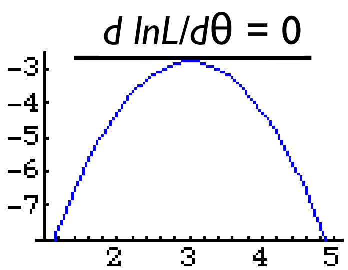
$$\ln L(x_1, x_2, \ldots, x_n|\theta) = \sum_{i=1}^{n} -\frac{1}{2}\ln(2\pi) - \frac{(x_i-\theta)^2}{2}$$

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

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

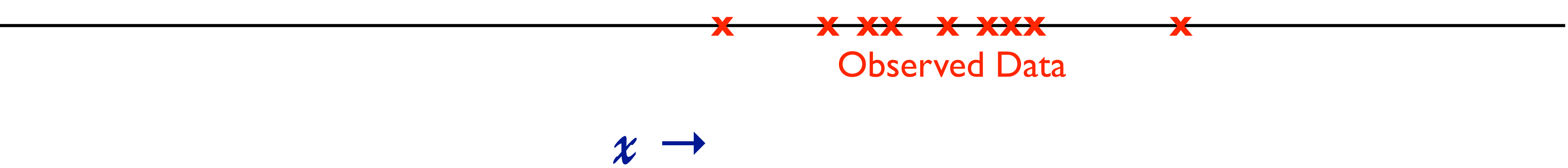
$$\boxed{\widehat{\theta} = \left(\sum_{i=1}^{n} x_i\right) / n = \overline{x}}$$

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



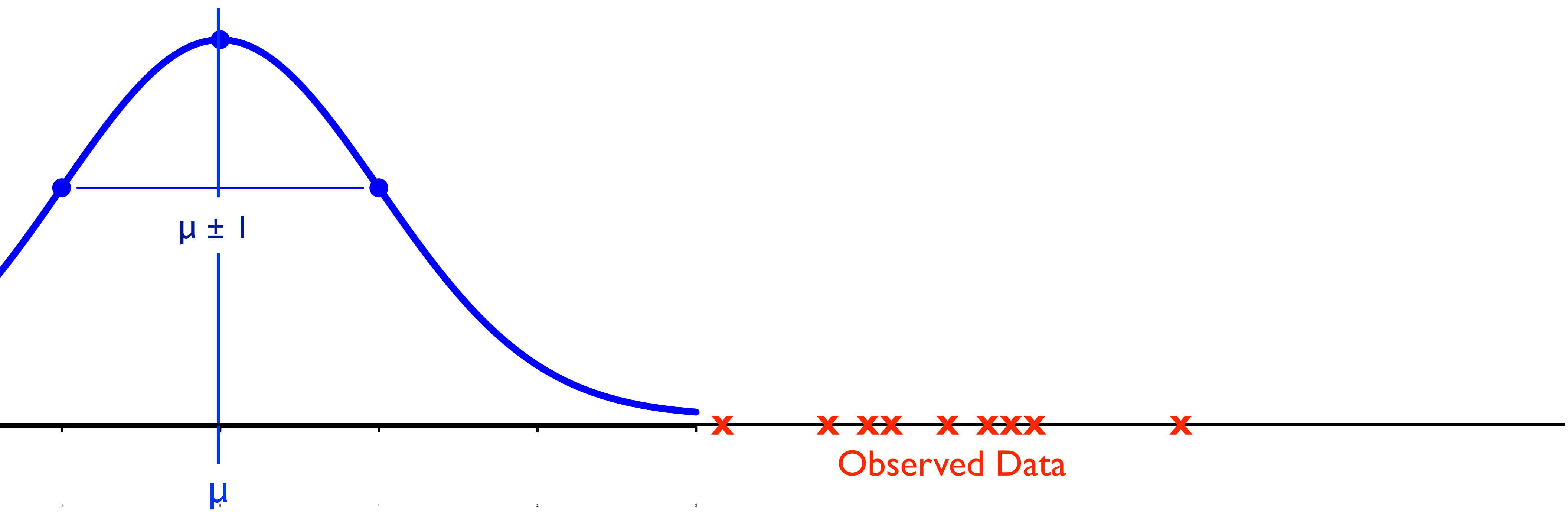
Sample mean is MLE of population mean

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



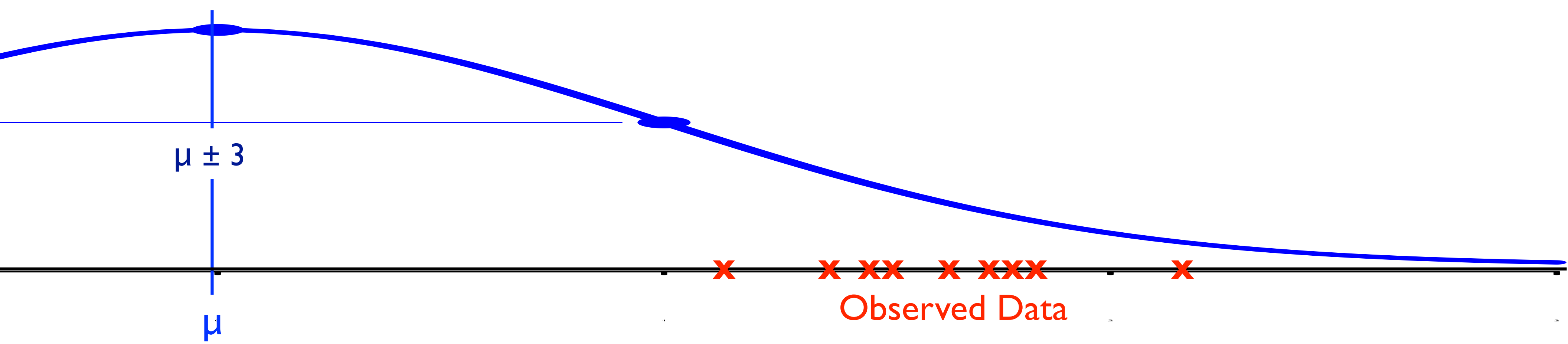
Which is more likely: (a) this?

μ, σ^2 both unknown



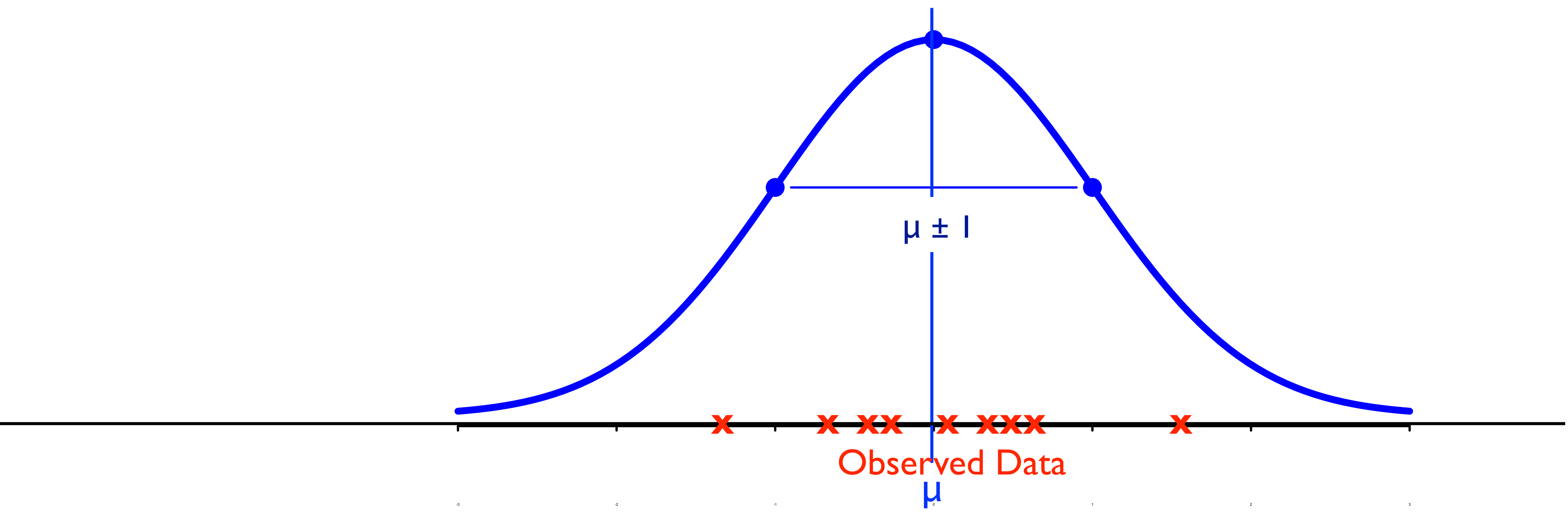
Which is more likely: (b) or this?

μ, σ^2 both unknown



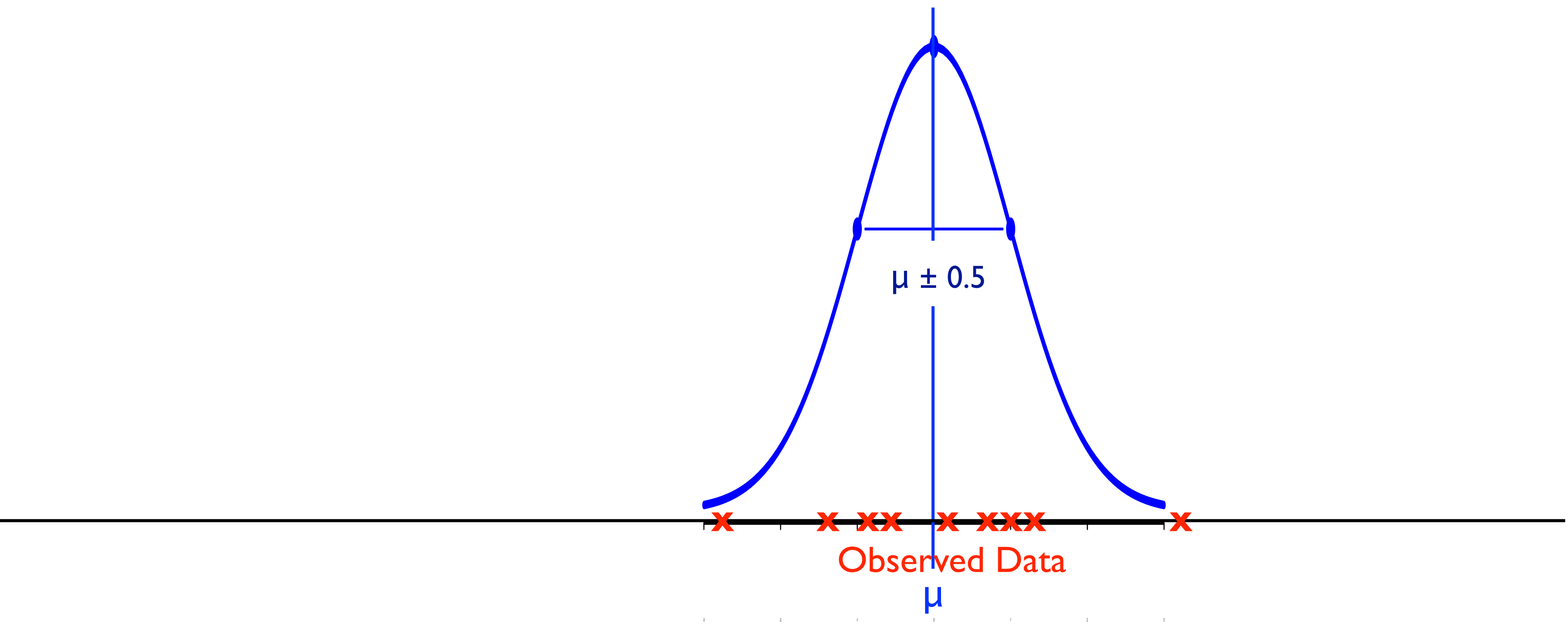
Which is more likely: (c) or this?

μ, σ^2 both unknown



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

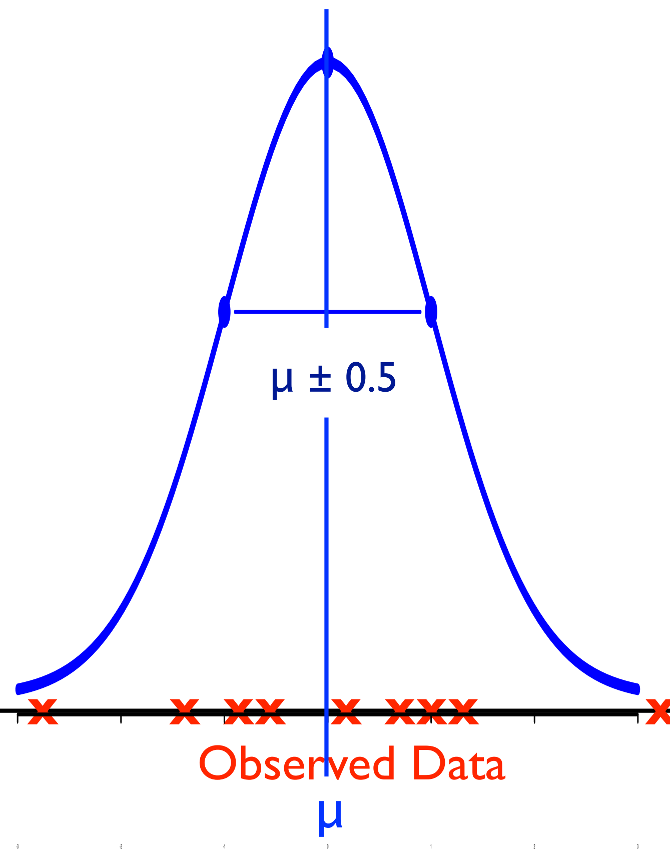
μ, σ^2 both unknown



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 & σ^2 ?

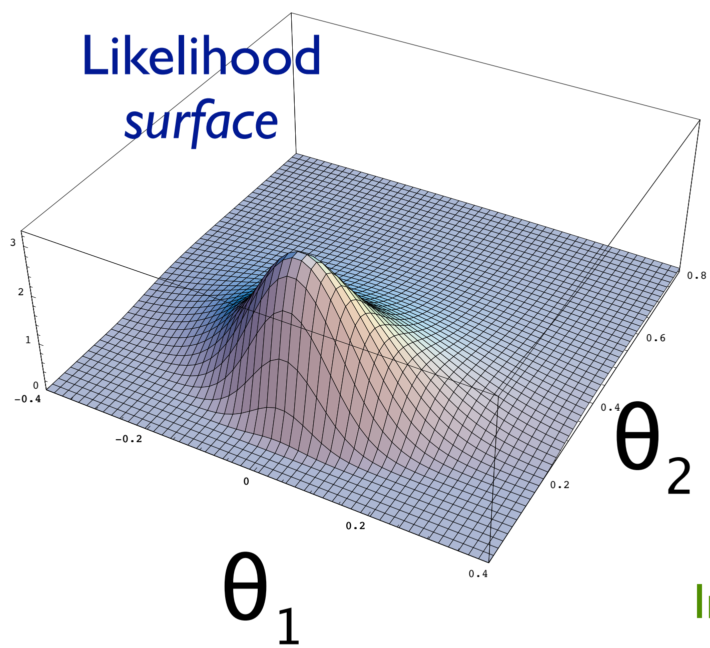


Ex 3: $x_i \sim N(\mu, \sigma^2)$, μ, σ^2 both unknown

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

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

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



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.)

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

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

$$\boxed{\widehat{\theta_2} \quad = \quad \left(\sum_{i=1}^{n}(x_i - \widehat{\theta}_1)^2\right)/n \quad = \quad \bar{s}^2}$$

Sample variance is MLE of *population* variance

Ex. 3, (cont.)

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

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

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

A consistent, but *biased* estimate of population variance.

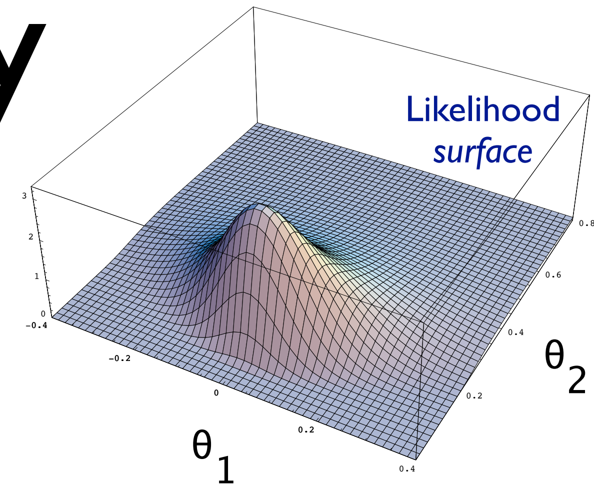
(An example of *overfitting.*) Unbiased estimate is:

I.e., $\lim_{n\to\infty}$ = correct

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

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

MLE 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

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"

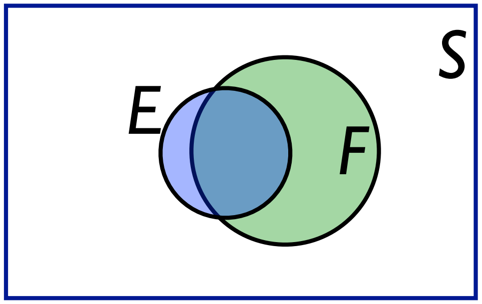
Of course, unusual samples will give bad estimates (estimate normal human heights from a sample of NBA stars?) but that is an unlikely event

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

Conditional Probability
&
Bayes Rule

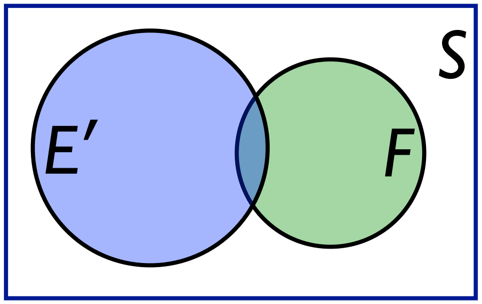
Conditional probability of E given F: probability that E occurs *given* that F has occurred.

"Conditioning on F"



Written as P(E|F)

Means "P(E has happened, given F observed)"

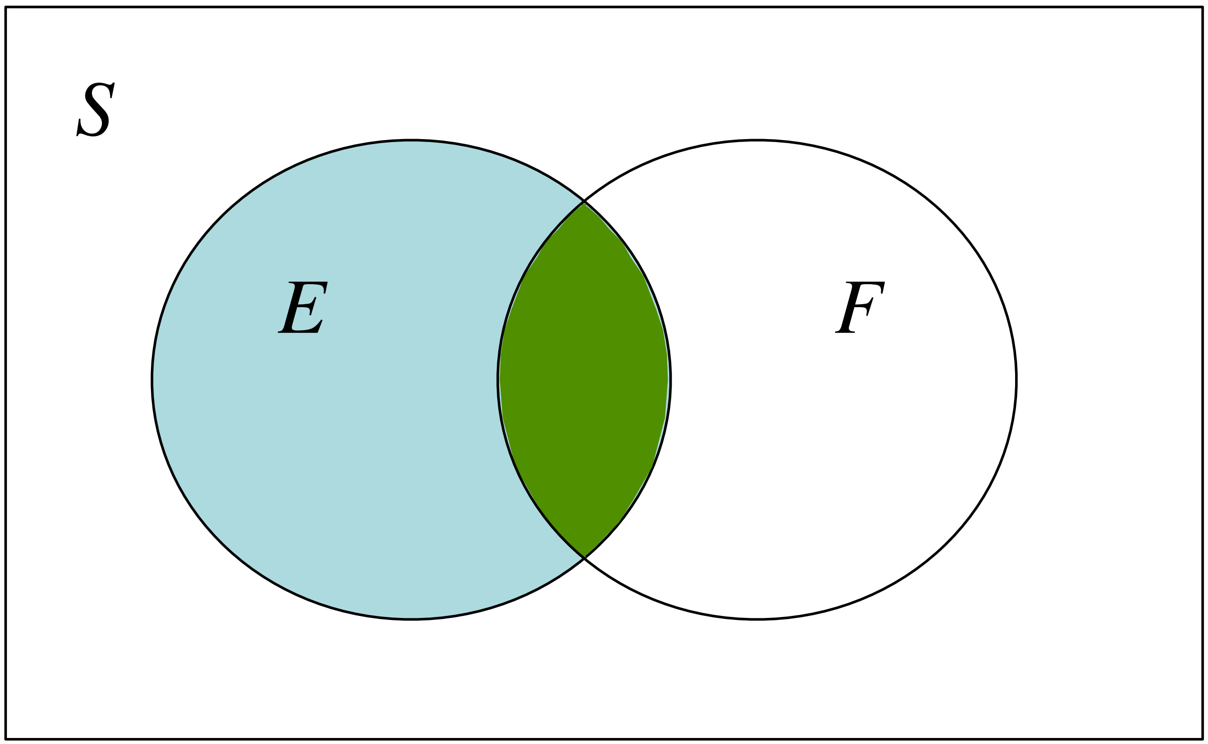


$$\boxed{P(E \mid F) = \frac{P(EF)}{P(F)}}$$ where P(F) > 0

$$P(EF) = P(E \mid F)\, P(F)$$

E and F are events in the sample space S

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



$$EF \cap EF^c = \varnothing$$

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

Most common form:

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

Expanded form (using law of total probability):

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

Proof:

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

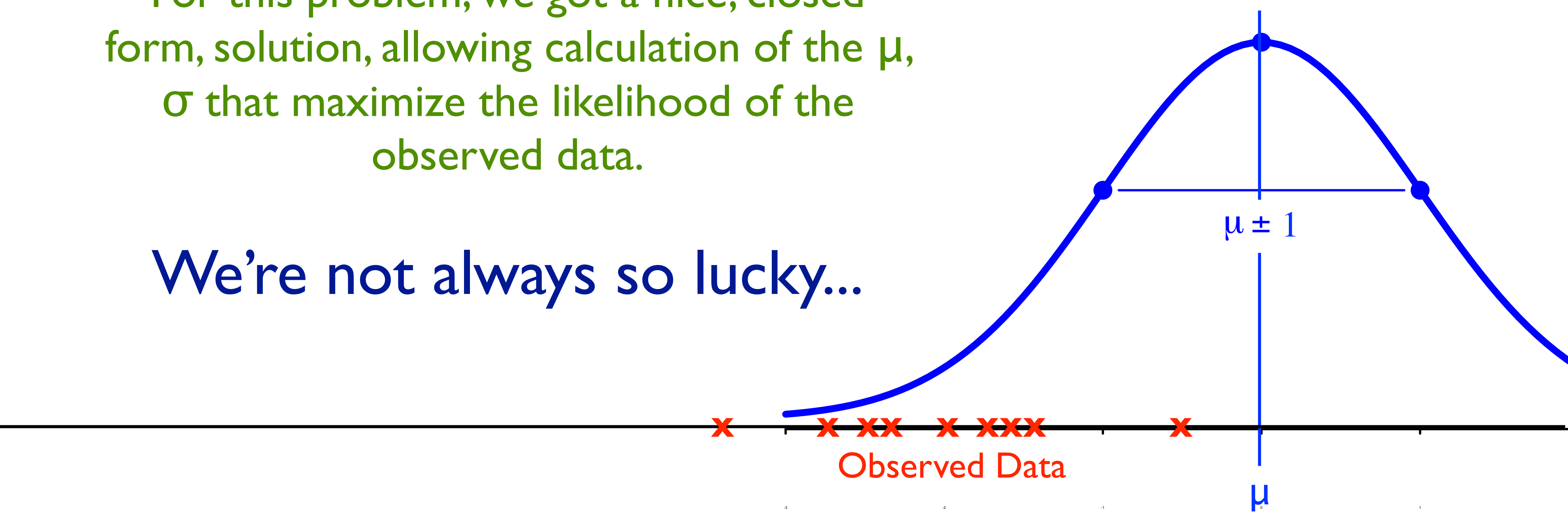
The "EM" Algorithm

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

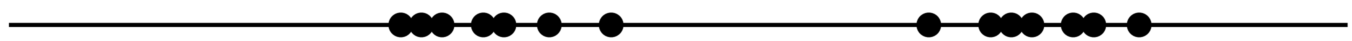
Previously:
How to estimate μ given data

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

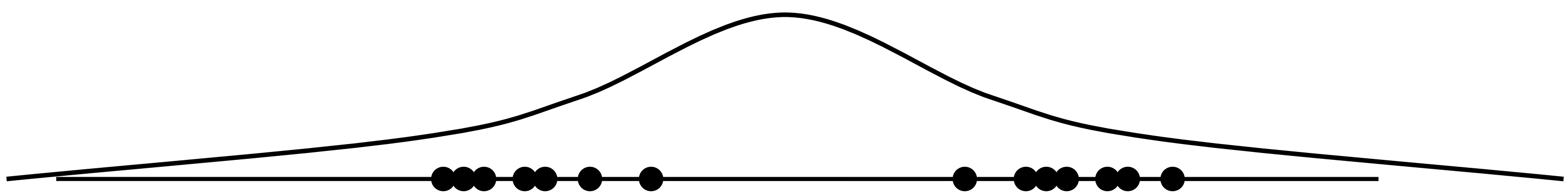
We're not always so lucky...



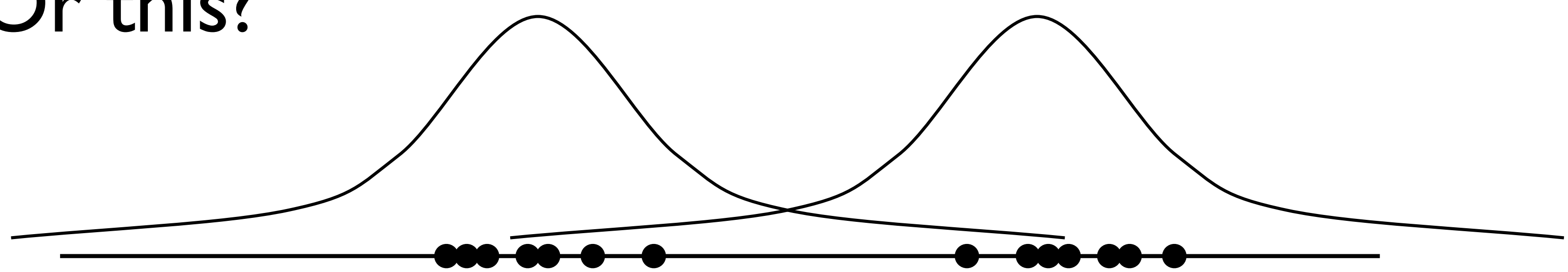
More Complex Example



This?

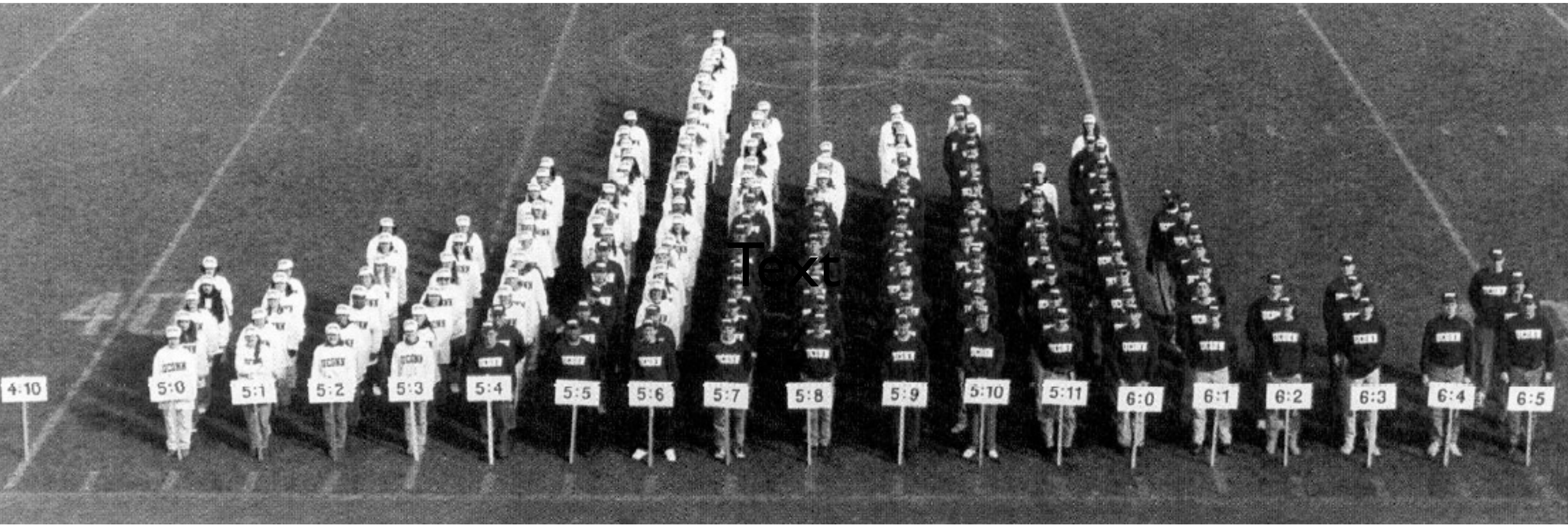


Or this?



(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

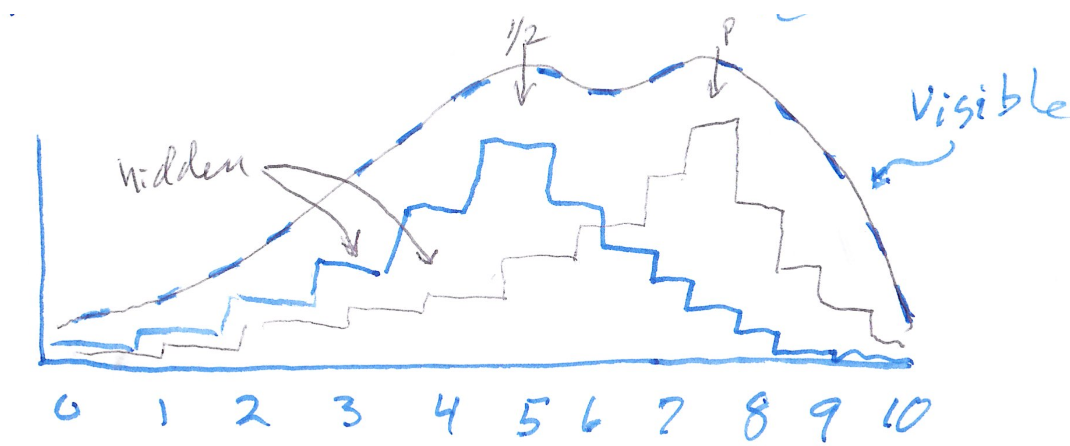
2 Coins: A Binomial Mixture

One fair coin (p(H)=1/2), and
one biased coin (p(H) = p, fixed but unknown)

For i = 1, 2, …, n:
  pick a coin at random,
  flip it 10 times
  record x_i = *# of heads*

What is MLE for p?

Expect histogram of x_i to look like:



EM as Chicken vs Egg

Hidden Data: let z_i = 1 if x_i was from biased coin, else 0

- *IF* I knew z_i, I could estimate p

  (easy: just use x_i s.t. z_i = 1)

- *IF* I knew p, I could estimate z_i

  (E.g., if $p = .8$, $x_i \geq 8$ implies z_i more likely 1;
  $x_i \leq 5$ implies z_i more likely 0;
  not clear-cut between, but uncertainty is quantifiable.)

Sadly, I know neither,
… but …

The "E-M Algorithm": iterate until convergence:

E-step: given (estimated) p, (re)-estimate z's

M-step: given (estimated) z's, (re)-estimate p

} Be Optimistic!

E = 0 • P(0) + 1 • P(1)

The E-Step

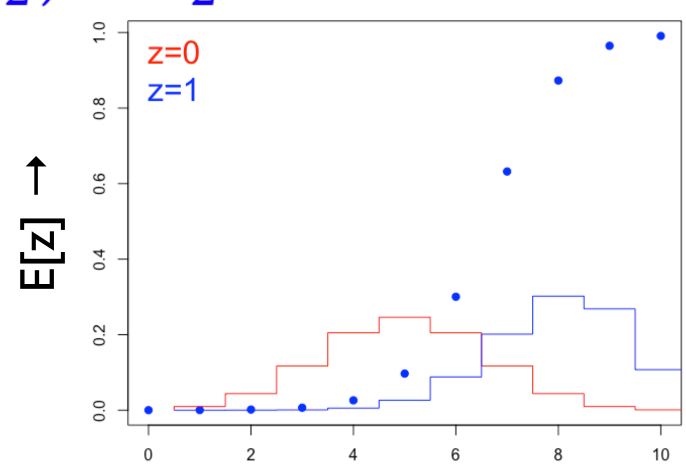
$$E[z_i] = Pr(z_i = 1 \mid x_i)$$

Bayes

$$= \frac{Pr(x_i \mid z_i = 1)Pr(z_i = 1)}{Pr(x_i \mid z_i = 1)Pr(z_i = 1) + Pr(x_i \mid z_i = 0)Pr(z_i = 0)}$$

$$= \frac{\binom{10}{x_i} \cdot p^{x_i}(1-p)^{10-x_i} \cdot \frac{1}{2}}{\binom{10}{x_i} \cdot p^{x_i}(1-p)^{10-x_i} \cdot \frac{1}{2} + \binom{10}{x_i} \cdot \left(\frac{1}{2}\right)^{10} \cdot \frac{1}{2}}$$

$$= \frac{p^{x_i}(1-p)^{10-x_i}}{p^{x_i}(1-p)^{10-x_i} + 2^{-10}}$$



Math-Hacking the "if "

Let $b(x \mid p)$ = binomial prob of x heads in 10 flips when p(H)=p

As above, z = 1 if x was biased, else 0

Then likelihood of x is

$L(x,z \mid p)$ = "if z == 1 then $b(x \mid p)$ else $b(x \mid ½)$"

Is there a smoother way? Especially, a differentiable way?

Yes! Idea #1:

$L(x,z \mid p) = z \cdot b(x \mid p) + (1-z) \cdot b(x \mid ½)$

Better still, idea #2:

$L(x,z \mid p) = b(x \mid p)^z \cdot b(x \mid ½)^{(1-z)}$

equal,
if
z is 0/1

The M-Step

"θ" here = "p" on previous slide

$$L(\vec{x}, \vec{z} \mid \theta) = C \prod_{i=1}^{n} \left(\theta^{x_i}(1-\theta)^{10-x_i}\right)^{z_i}, \text{ where } C = \prod_{i=1}^{n} \binom{10}{x_i} \left(\frac{1}{2^{10}}\right)^{1-z_i}$$

$$E[\log L(\vec{x}, \vec{z} \mid \theta)] = E\left[\log C + \sum_{i=1}^{n} z_i(x_i \log\theta + (10-x_i)\log(1-\theta))\right]$$

$$= E[\log C] + \sum_{i=1}^{n} E[z_i](x_i \log\theta + (10-x_i)\log(1-\theta))$$

linearity of expectation

$$\frac{d}{d\theta} E[\log L(\vec{x}, \vec{z} \mid \theta)] = 0 + \sum_{i=1}^{n} E[z_i]\left(\frac{x_i}{\theta} - \frac{10-x_i}{1-\theta}\right)$$

Set to zero and solve, using $E[z_i] = \widehat{z_i}$ from E-step. Result (after some algebra):

$$\boxed{\widehat{\theta} = \frac{\sum_{i=1}^{n} \widehat{z_i} \cdot x_i}{\sum_{i=1}^{n} \widehat{z_i} \cdot 10}}$$

Intuitively sensible: the estimated fraction of heads from the biased coin is the observed fraction of heads seen overall, after *weighting* by the probability that each observation was indeed from the biased coin.

Suggested exercise(s)

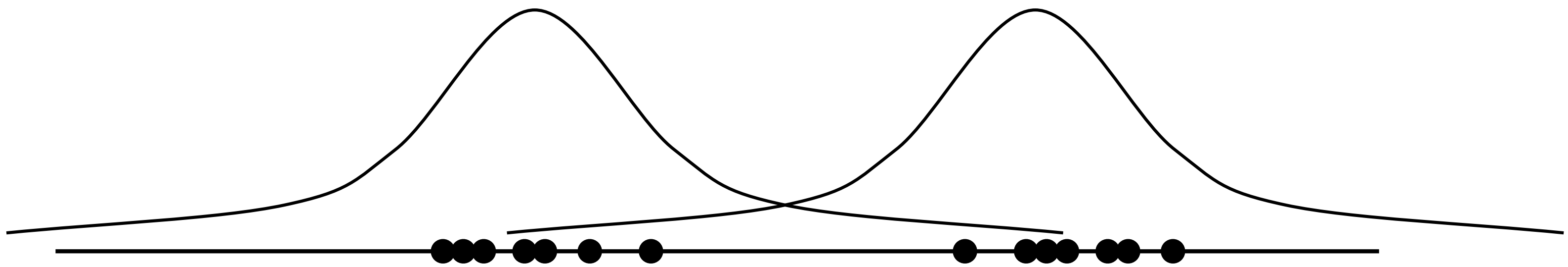
Redo the math assuming *both* coins are biased (but unequally)

Write code to implement either version

Or a spreadsheet, with "fill down" to do a few iterations

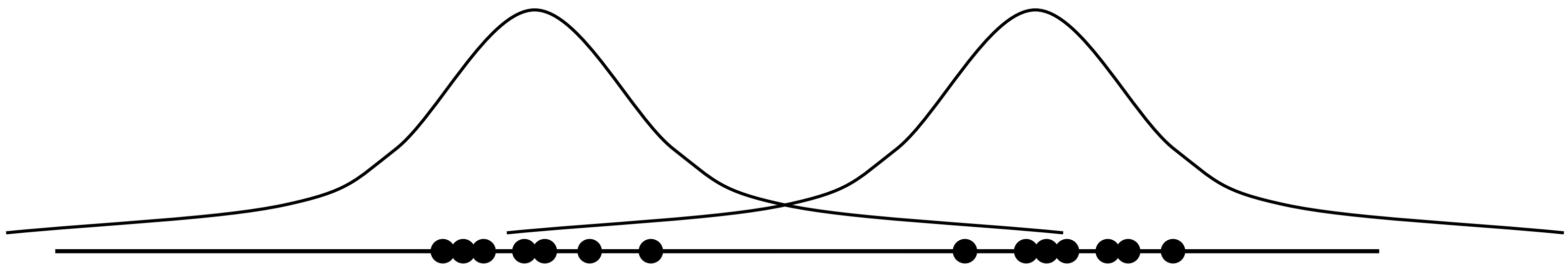
Even in the 1-coin-biased version, there may be multiple local maxima (e.g., consider histogram with a small peak at .25 and large ones at .5 & .8) Does your alg get stuck at local max? How often? Does random restart pragmatically fix this?

EM for a Gaussian Mixture



I have presented the Gaussian mixture example in other courses. I will *NOT* lecture on it in 427, but I'll leave the slides (46-58) here in case you are interested in seeing another example in detail. Happy to discuss in office hours.

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

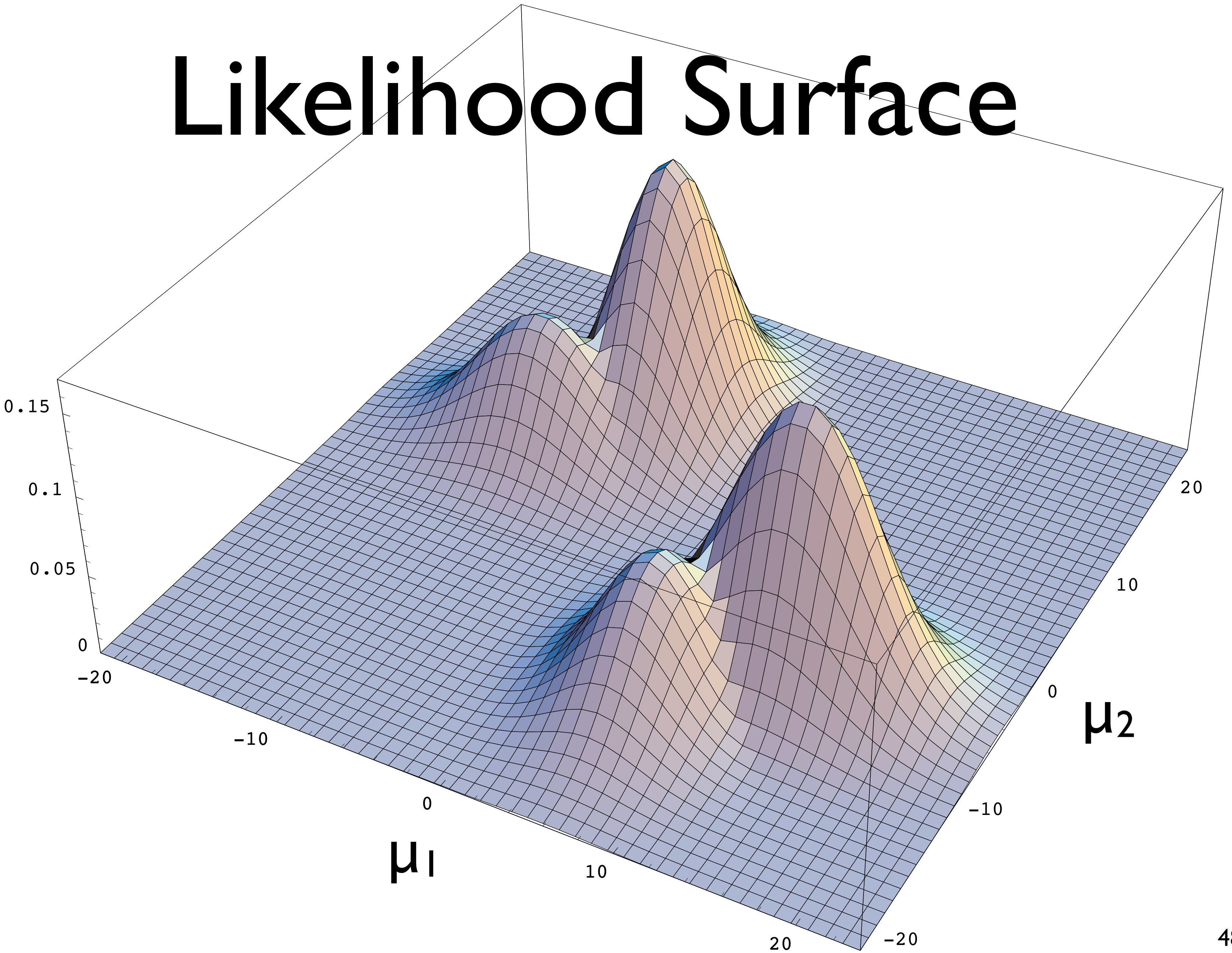
$\xrightarrow{\text{together}}$ $\boxed{\tau_1 f(x|\mu_1, \sigma_1^2) + \tau_2 f(x|\mu_2, \sigma_2^2)}$

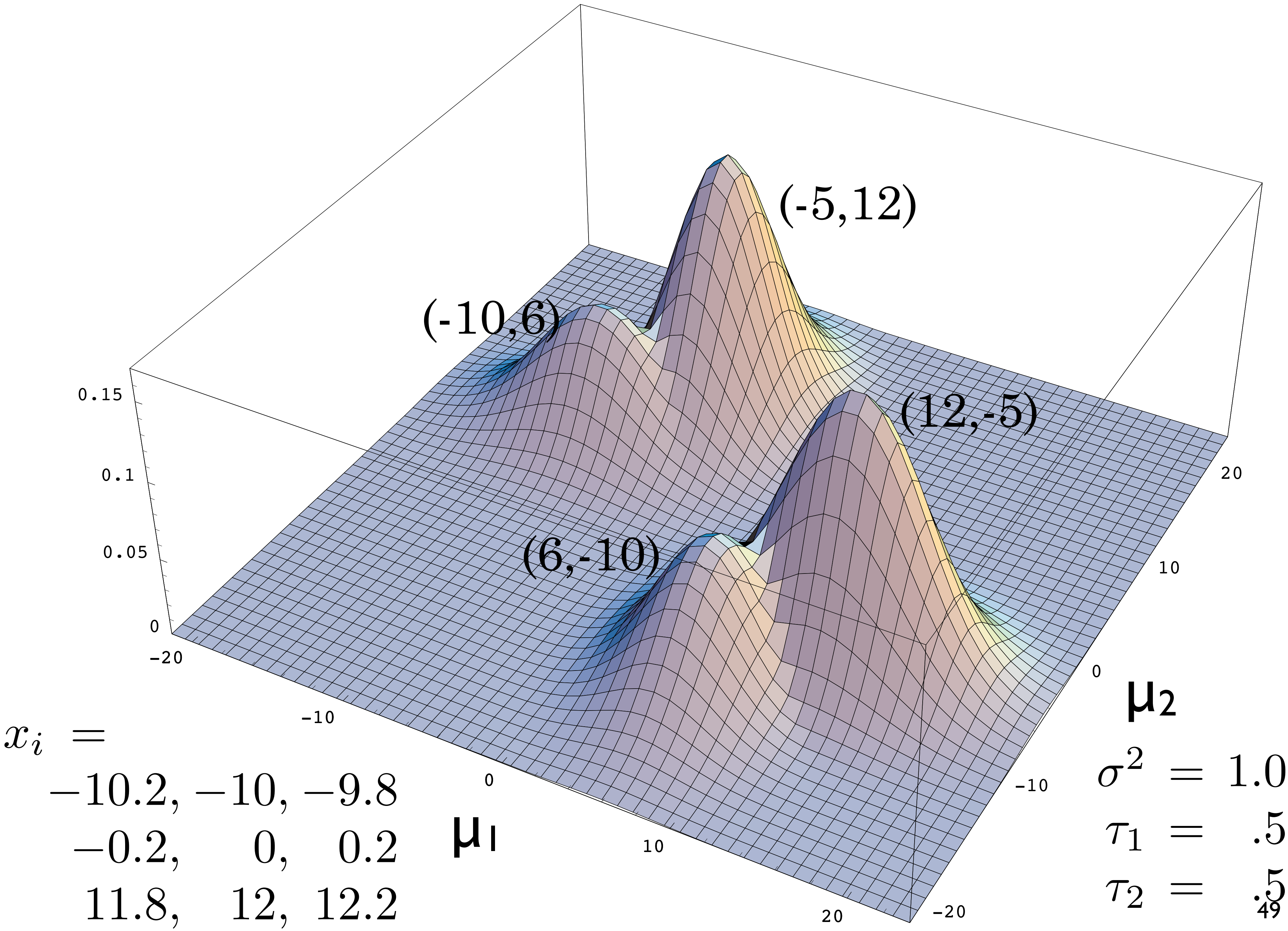
Likeli-hood

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

No closed-form max

Likelihood Surface




(-5,12)
(-10,6)
(12,-5)
(6,-10)
0.15
0.1
0.05
0
-20
-10
0
10
20
μ_1
μ_2
$x_i =$
$-10.2, -10, -9.8$
$-0.2, 0, 0.2$
$11.8, 12, 12.2$
$\sigma^2 = 1.0$
$\tau_1 = .5$
$\tau_2 = .5$

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

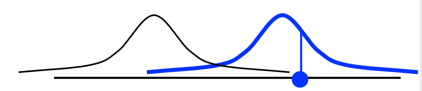
But *what if* we knew the *hidden data*?

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

EM as Egg vs Chicken

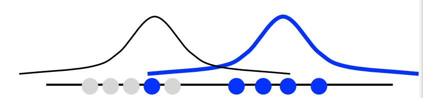
IF parameters θ known, could estimate z_{ij}

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



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:

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

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

Overall, a clever "hill-climbing" strategy

Not "EM," 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.

"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)

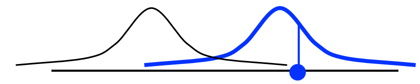
But z_{ij}'s aren't known.

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)

I.e., average over possible, but hidden 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)

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

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

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

Repeat for each $z_{i,j}$

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

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

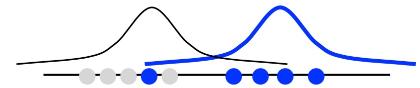
Formulas with "if's" are messy; can we blend more smoothly?
Yes, many possibilities. Idea 1:

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

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)

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, maximum likelihood parameter estimation; broader than just these examples

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

Iterate:

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

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

EM Issues

Under mild assumptions (e.g., 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, esp. with *random restarts*