CSE 527

Autumn 2009

4: MLE, EM

FYI: Hemo-globin History

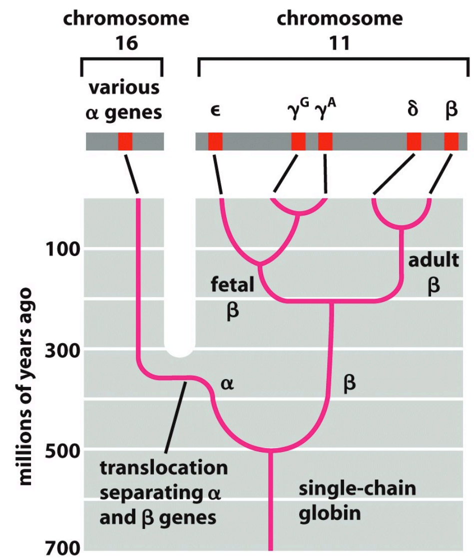

Figure 4-87 Molecular Biology of the Cell 5/e (© Garland Science 2008)

Browser

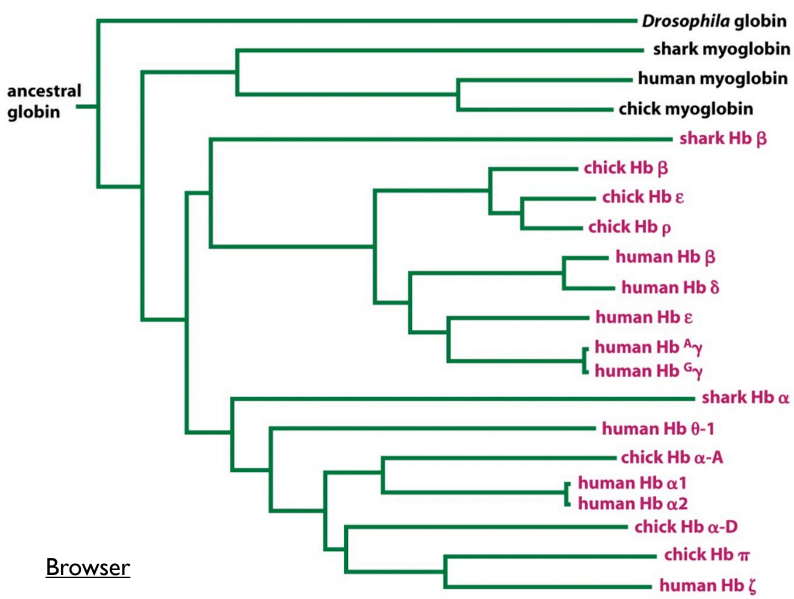

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Figure 1-26 Molecular Biology of the Cell 5/e (© Garland Science 2008)

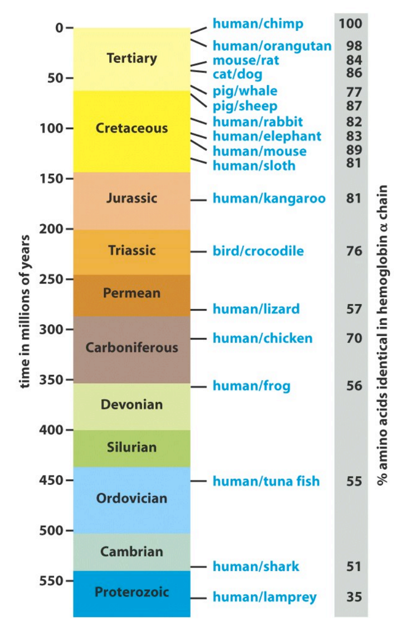


Figure 1-52 Molecular Biology of the Cell 5/e (© Garland Science 2008)

Outline

MLE: Maximum Likelihood Estimators

EM: the Expectation Maximization Algorithm

Next: Motif description & discovery

Learning From Data: MLE

Maximum Likelihood Estimators

Probability Basics, I

	Ex.	Ex.
Sample Space	$\{1, 2, \ldots, 6\}$	$\mathbb{R}$
Distribution	$p_1, \ldots, p_6 \geq 0; \sum_{1 \leq i \leq 6} p_i = 1$	$f(x) >= 0; \int_{\mathbb{R}} f(x)dx = 1$
e.g.	$p_1 = \cdots = p_6 = 1/6$	$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/(2\sigma^2)}$

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

Parameter Estimation

Assuming sample $x_1, x_2, ..., x_n$ is from a parametric distribution $f(x|\theta)$, estimate θ.

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

θ = probability of Heads

Likelihood

P(x | θ): Probability of event x given model θ

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

E.g., Σ_x P(x | θ) = 1

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

E.g., Σ_θ P(x | θ) can be anything; *relative* values of interest.

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

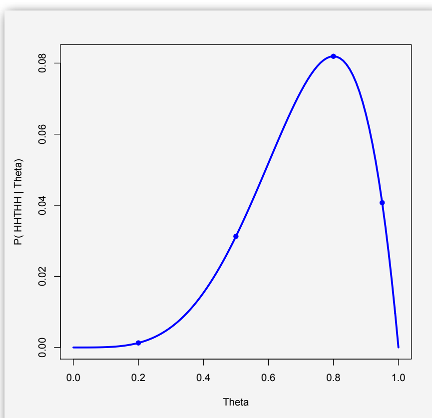
I.e., event HHTHH is *more likely* when θ = .6 than θ = .5

And what θ make HHTHH *most* likely?

Likelihood Function

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 $x_1, x_2, ..., x_n$

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

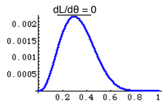
As a function of θ, what θ maximizes the likelihood of the data actually observed

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 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:

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

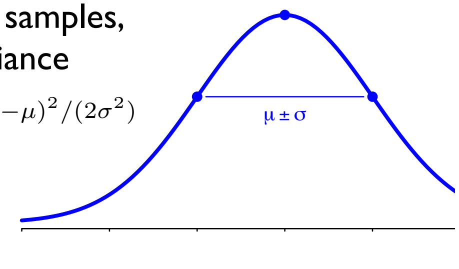
Observed fraction of successes in sample is MLE of success probability in population

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

Parameter Estimation

Assuming sample $x_1, x_2, ..., x_n$ is from a parametric distribution $f(x|\theta)$, estimate θ.

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

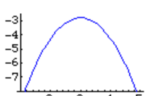


$$\begin{aligned} f(x) &= \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/(2\sigma^2)} \\ \theta &= (\mu, \sigma^2) \end{aligned}$$

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

$$\begin{aligned} L(x_1, x_2, \ldots, x_n|\theta) &= \prod_{1\le i\le n} \frac{1}{\sqrt{2\pi}} e^{-(x_i-\theta)^2/2} \\ \ln L(x_1, x_2, \ldots, x_n|\theta) &= \sum_{1\le i\le n} -\frac{1}{2}\ln 2\pi - \frac{(x_i-\theta)^2}{2} \\ \frac{d}{d\theta} \ln L(x_1, x_2, \ldots, x_n|\theta) &= \sum_{1\le i\le n} (x_i - \theta) \\ &= \left(\textstyle\sum_{1\le i\le n} x_i\right) - n\theta = 0 \end{aligned}$$

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

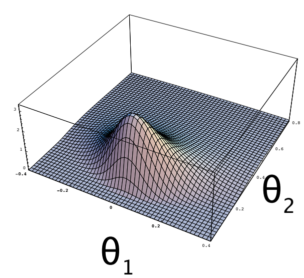


$$\boxed{\hat\theta = \left(\textstyle\sum_{1\le i\le n} x_i\right)/n = \bar{x}}$$

Sample mean is MLE of population mean

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

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



$$\boxed{\hat\theta_1 = \left(\textstyle\sum_{1\le i\le n} x_i\right)/n = \bar{x}}$$

Sample mean is MLE of population mean, again

Ex. 3, (cont.)

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

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

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

A consistent, but *biased* estimate of population variance. (An example of *overfitting.)* Unbiased estimate is:

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

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

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

Aside: Is it Biased? Why?

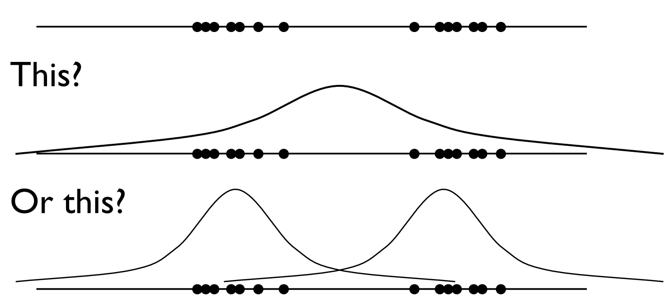
Is it? Yes. As an extreme, when n = 1, $\hat{\theta}_2 = 0$.

Why? A bit harder to see, but think about n = 2. Then $\hat{\theta}_1$ is exactly between the two sample points, the position that exactly minimizes the expression for $\hat{\theta}_2$. Any other choices for θ_1, θ_2 make the likelihood of the observed data slightly lower. But it's actually pretty unlikely that two sample points would be chosen exactly equidistant from, and on opposite sides of the mean, so the MLE $\hat{\theta}_2$ systematically underestimates θ_2.

EM

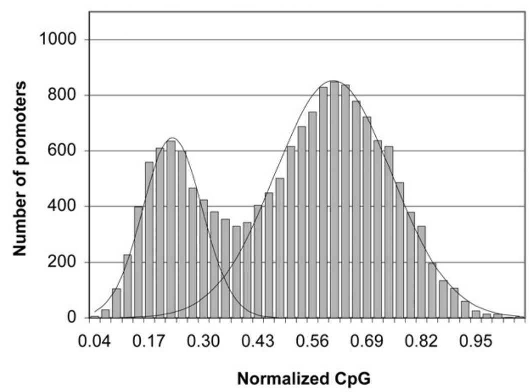
The Expectation-Maximization Algorithm

More Complex Example



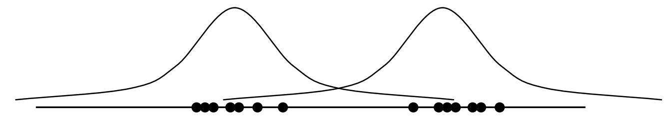
(A modeling decision, not a math problem..., but if later, what math?)

A Real Example:
CpG content of human gene promoters



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

Gaussian Mixture Models / Model-based Clustering



Parameters θ

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

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

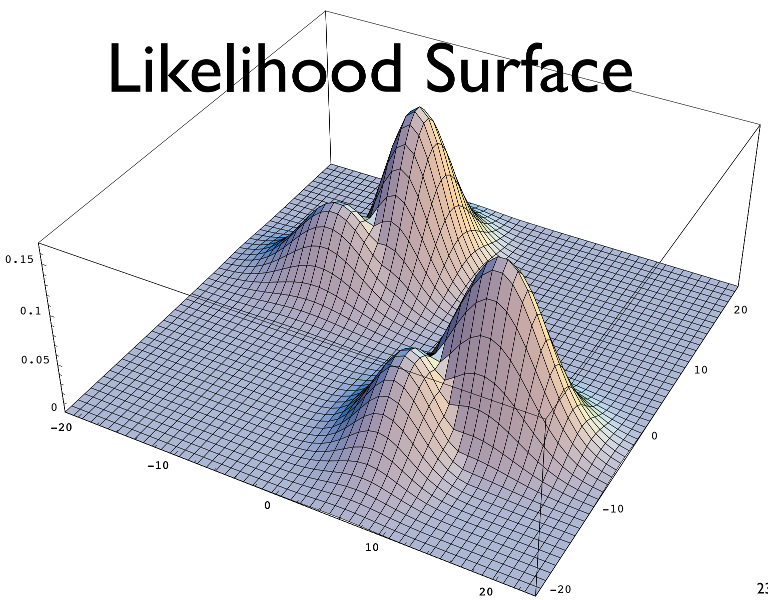
Likelihood

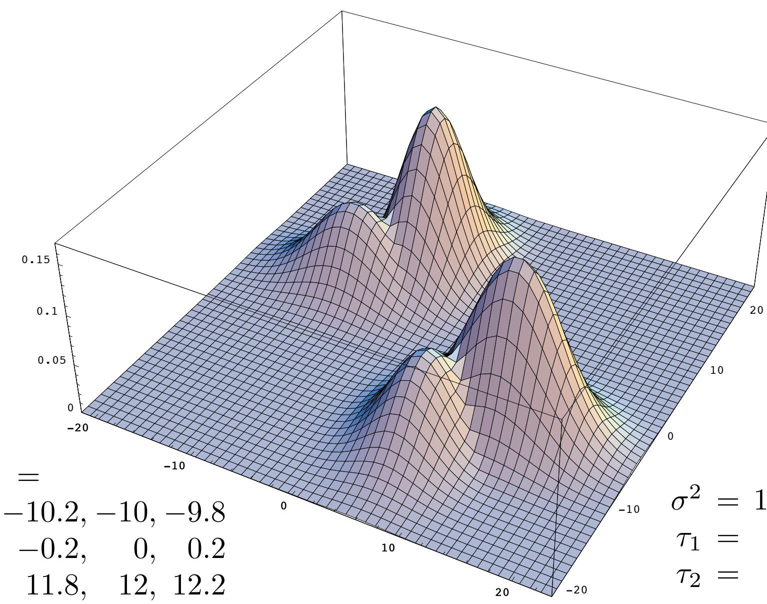
$$L(x_1, x_2, \ldots, x_n | \mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \tau_1, \tau_2)$$

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

No closed-form max

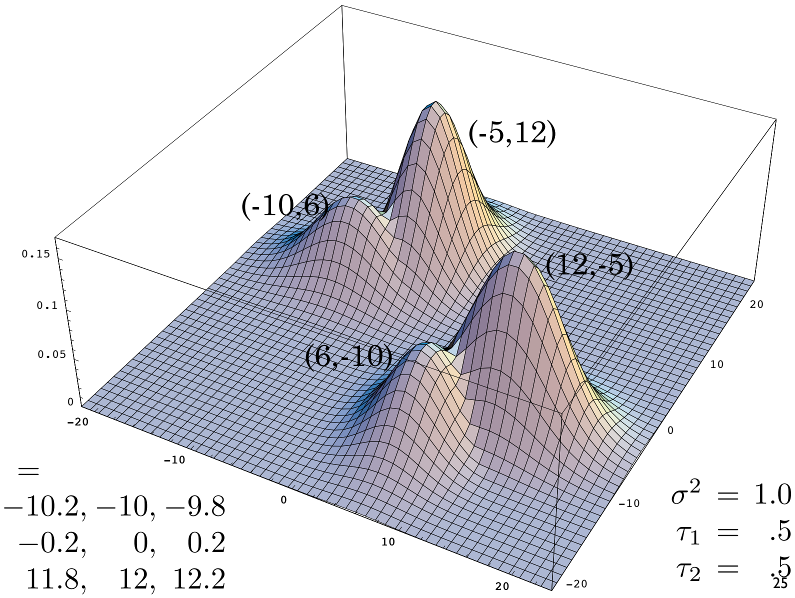
Likelihood Surface





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

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



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$11.8, \quad 12, \quad 12.2$

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

A What-If Puzzle

Likelihood

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

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

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

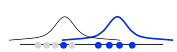
But *what if* we knew the *hidden data?*

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

EM as Egg vs Chicken

IF z_{ij} known, could estimate parameters θ

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



IF parameters θ known, could estimate z_{ij}

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

But we know neither; (optimistically) iterate:

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

Overall, a clever "hill-climbing" strategy

Simple Version: "Classification EM"

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

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

Now recalc θ, assuming that partition

Then recalc z_{ij}, assuming that θ

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

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

Full EM

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

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

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

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

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

Instead, maximize *expected* likelihood of visible data

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

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

The E-step:

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

Assume θ known & fixed

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

D: the observed datum x_i

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

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

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

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

Repeat for each x_i

Complete Data Likelihood

Recall:

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

so, correspondingly,

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

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

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

Idea 2 (Better):

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

M-step:

Find θ maximizing E(log(Likelihood))

(For simplicity, assume $\sigma_1 = \sigma_2 = \sigma; \tau_1 = \tau_2 = .5 = \tau$)

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

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

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

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

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

2 Component Mixture

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

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

EM Summary

Fundamentally a max likelihood parameter estimation problem

Useful if analysis is more tractable when 0/1 hidden data z known

Iterate:

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

EM Issues

Under mild assumptions (sect 11.6), EM is guaranteed to increase likelihood with every E-M iteration, hence will converge.

But may converge to *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