

Algorithm Foundations of Data Science and Engineering

Lecture 13: EM Algorithm

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Outline

Motivation

Likelihood

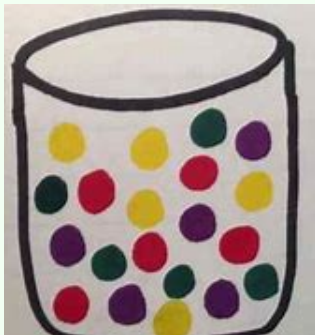
EM Algorithm

- Motivation

- Mixture Models

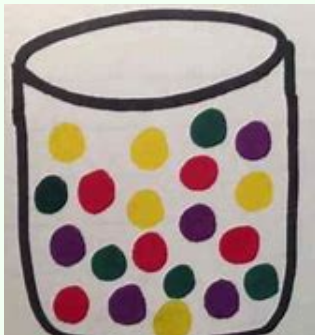
- EM Algorithm

A probabilistic game



There are 6 balls in a bag, 3 are red, 2 are yellow and 1 is blue. What is the probability of picking a yellow?

A probabilistic game



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- If we pick 20 times, we obtain 5 red, 12 yellow, and 3 blue;

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- If we pick 20 times, we obtain 5 red, 12 yellow, and 3 blue;
- Do you believe there are 3 are red, 2 are yellow and 1 is blue balls in the bag?

A probabilistic game



There are 6 balls in a bag, 3 are red, 2 are yellow and 1 is blue. What is the probability of picking a yellow?

- If we pick 20 times, we obtain 5 red, 12 yellow, and 3 blue;
- Do you believe there are 3 are red, 2 are yellow and 1 is blue balls in the bag?
- How about 2 are red, 3 are yellow and 1 is blue?

Intuition of likelihood



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If we toss an unfair coin 10 times, the result is

$T, T, T, H, T, T, T, H, T, T.$

Would you guess the probability $P(H)$?

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Would you guess the probability $P(H)$?

- We wish to fit the parameters of a model $p(x; \theta)$ to the data;

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Would you guess the probability $P(H)$?

- We wish to fit the parameters of a model $p(x; \theta)$ to the data;
- We can infer the parameter via maximizing the joint probability that observes the above sample.

Definition of likelihood

Suppose that sample point X_1, X_2, \dots, X_n have a joint density or pmf $f(x_1, x_2, \dots, x_n | \theta)$. Given observe value of $X_i = x_i$, the **likelihood** of θ as a function of x_1, x_2, \dots, x_n is defined as

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- The method of maximum likelihood can be applied to a great variety of other statistical problems, such as curve fitting, testing, and machine learning, etc.
- Maximum likelihood estimates have nice theoretical properties as well.

Maximum likelihood estimator

Definition

For each sample point \mathbf{x} , let $\hat{\theta}(\mathbf{x})$ be a parameter value at which $L(\theta|\mathbf{x})$ attains its maximum as a function of θ , with \mathbf{x} held fixed. That is,

$$\hat{\theta}(\mathbf{x}) = \operatorname{argmax}_{\theta} L(\theta|\mathbf{x}).$$

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- The MLE is the parameter point for which the observed sample is most likely.
- There are two drawbacks:
 - It is actually to find the global maximum. In many cases, this problem reduces to a simple differential calculus exercise but, sometimes even for common densities, difficulties do arise.
 - It is numerical sensitivity.

How to obtain the maximum likelihood estimator

If the likelihood function is differentiable (in θ_i), possible candidates for the MLE are the values of $(\theta_1, \dots, \theta_k)$ that solve

$$\frac{\partial}{\partial \theta_i} L(\theta|\mathbf{x}) = 0, i = 1, \dots, k.$$

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- The zeros of the first derivative locate only extreme points in the interior of the domain of a function.
- If the extrema occur on the boundary the first derivative may not be 0.
- Thus, the boundary must be checked separately for extrema.

Poisson MLE

Let X_1, X_2, \dots, X_n be i.i.d. Poisson sample $\frac{\lambda^x}{x!} e^{-\lambda}$, and let $L(\lambda|\mathbf{x})$ denote the likelihood function. Then

$$\log L(\lambda|\mathbf{x}) = \sum_{i=1}^n (X_i \log \lambda - \lambda - \log X_i!) = \log \lambda \sum_{i=1}^n X_i - n\lambda - \sum_{i=1}^n \log(X_i!)$$

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which has the solution $\hat{\lambda} = \bar{x}$.

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- We can verify that $\frac{d^2}{d\theta^2} L(\theta|\mathbf{x})|_{\theta = \bar{x}} < 0$. Thus \bar{x} is the only extreme point in the interior and it is a maximum.
- By taking limits it is easy to establish that the likelihood is 0 at $\pm\infty$.

Therefore, $\hat{\theta} = \bar{x}$ is a global maximum and \bar{X} is the MLE.

Normal MLE

Let X_1, X_2, \dots, X_n be i.i.d. $N(\mu, \sigma)$, and let $L(\theta|\mathbf{x})$ denote the likelihood function. Then

$$\log L(\mu, \sigma|\mathbf{x}) = -n \log \sigma - \frac{n}{2} \log 2\pi - \frac{1}{2\sigma^2} \sum_{i=1}^n (X_i - \mu)^2$$

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The equations $\frac{\partial}{\partial \mu} \log L(\mu, \sigma|\mathbf{x}) = 0$ and $\frac{\partial}{\partial \sigma} \log L(\mu, \sigma|\mathbf{x}) = 0$ reduce to

$$\frac{1}{\sigma^2} \sum_{i=1}^n (x_i - \mu) = 0 \text{ and } -\frac{n}{\sigma} + \sigma^{-3} \sum_{i=1}^n (x_i - \mu)^2 = 0$$

which has the solution

$$\hat{\mu} = \bar{x} \text{ and } \hat{\sigma} = \sqrt{\frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2}$$

Normal MLE Cont'd

Recall that for any number a ,

$$\sum_{i=1}^n (x_i - a)^2 \geq \sum_{i=1}^n (x_i - \bar{x})^2$$

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

with equality if and only if $\theta = \bar{x}$. Hence \bar{X} is the MLE.

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In most cases, especially when differentiation is to be used, it is easier to work with the natural logarithm of $L(\theta|\mathbf{x})$, $\log L(\theta|\mathbf{x})$ (known as the **log likelihood**), than it is to work with $L(\theta|\mathbf{x})$ directly.

Bernoulli MLE

Let X_1, X_2, \dots, X_n be i.i.d. $Bernoulli(p)$. Then the log likelihood function is

$$l(p|\mathbf{x}) = y \log p + (n - y) \log (1 - p).$$

where $y = \sum_{i=1}^n x_i$.

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$$\log L(p|\mathbf{x}) = \begin{cases} n \log (1 - p), & \text{if } y = 0 \\ n \log p, & \text{if } y = n \end{cases}$$

In either case $l(p|\mathbf{x})$ is a monotone function of p , and it is again straightforward to verify that $\hat{p} = \frac{1}{n} \sum_{i=1}^n x_i$ in each case.

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In either case $l(p|\mathbf{x})$ is a monotone function of p , and it is again straightforward to verify that $\hat{p} = \frac{1}{n} \sum_{i=1}^n x_i$ in each case. Thus, we have shown that $\frac{1}{n} \sum_{i=1}^n x_i$ is the MLE of p .

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EM algorithm: the intuition



H T T T H H T H T H



H H H H T H H H H H



H T H H H H H T H H








H T H T T T H H T T



T H H H T H H H T H

Coin A	Coin B
	5 H, 5 T
9 H, 1 T	
8 H, 2 T	
	4 H, 6 T
7 H, 3 T	
24 H, 6 T	9 H, 11 T






EM algorithm: the intuition

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Assume that we have two coins, A and B






EM algorithm: the intuition

- Assume the bias of A is θ_1 (i.e., probability of getting heads with A);

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Assume a more challenging problem:

EM algorithm: the intuition



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- We want to find the values of θ_1 and θ_2 .

Assume that we have two coins, A and B

Assume a more challenging problem: we do not know the identities of the coins used for each set of tosses (we treat them as hidden variables).

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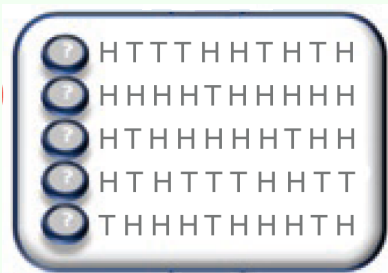
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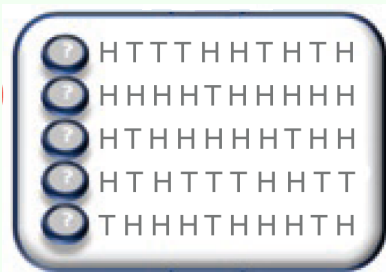
$$\hat{\theta}_1 = \frac{\# \text{ heads using } A}{\# \text{ flips using } A} \quad ?$$

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The parameters of the model cannot be estimated. Thus, it becomes a more challenging problem.

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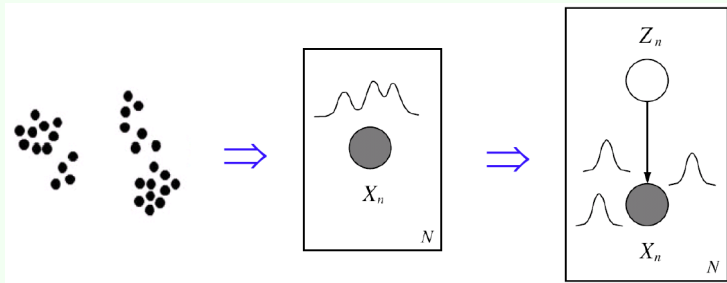
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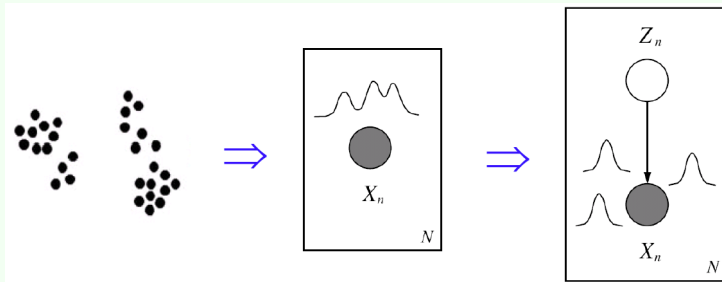
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Discrete latent variables can be used to partition/cluster data into sub-groups (mixture models).

Mixed models

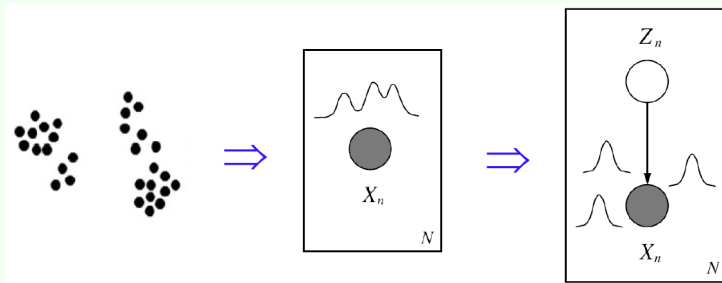


Mixed models



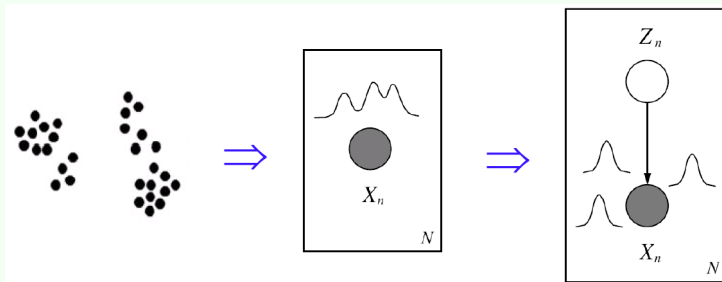
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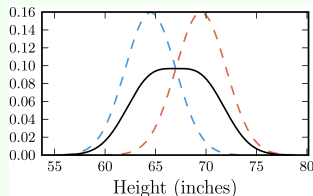
- A density model $p(x)$ may be multi-modal;
- We may be able to model it as a mixture of uni-modal distributions (e.g., Bernoulli or Gaussians, etc).
- Each mode may correspond to a different sub-population (e.g., male and female).

Gaussian mixture models (GMMs)

For example, the height of a randomly chosen man is normally distributed with a mean around 5'9.5" and standard deviation around 2.5". Similarly, the height of a randomly chosen woman is normally distributed with a mean around 5'4.5" and standard deviation around 2.5". Is the height of a randomly chosen person normally distributed?

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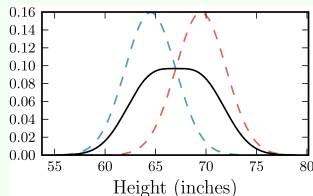
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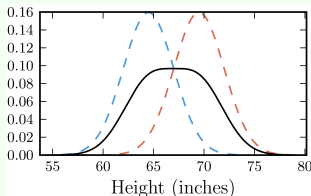
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The answer is no.



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The answer is no. This one is a little more deceptive: because there's so much overlap between the height distributions for men and for women, the overall distribution is in fact highest at the center. But it's still not normally distributed: it's too wide and at in the center (we'll formalize this idea in just a moment).

GMM

Formally, suppose we have people numbered $i = 1, \dots, n$. We observe r.v. $Y_i \in \mathcal{R}$ for each person's height, and assume there is an unobserved label $C_i \in \{M, F\}$ for each person representing that person's gender, where c stands for "class". Assume that the two groups have the same known variance σ^2 , but different unknown means μ_M and μ_F .

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The conditional distribution within each class is Gaussian:

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There is no way we can solve this in closed form.

Outline

Motivation

Likelihood

EM Algorithm

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Mixture Models

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However, if we had some way of completing the data (in our case, guessing correctly which coin was used in each of the five sets), then we could reduce parameter estimation for this problem with incomplete data to maximum likelihood estimation with complete data.

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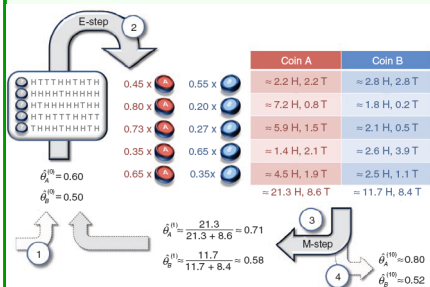
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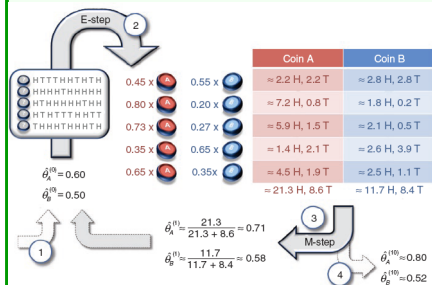
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The expectation maximization algorithm (EM algorithm) is a refinement on this basic idea.

Refinement



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$$P(A|Y)$$

$$= \frac{P(Y|A)P(A)}{P(Y|A)P(A) + P(Y|B)P(B)}$$

$$= \frac{0.24^5 \cdot P(A)}{0.24^5 \cdot P(A) + 0.25^5 \cdot P(B)}$$

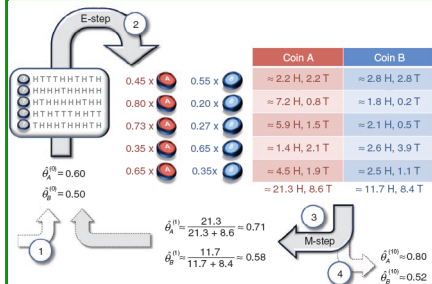
$$= \frac{7962624}{7962624 + 9765625} \approx 0.45$$

$$P(B|Y) = 1 - P(A|Y) = 0.55$$

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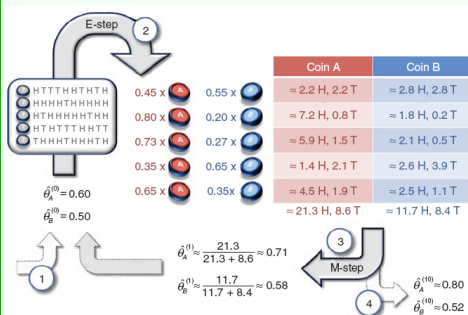
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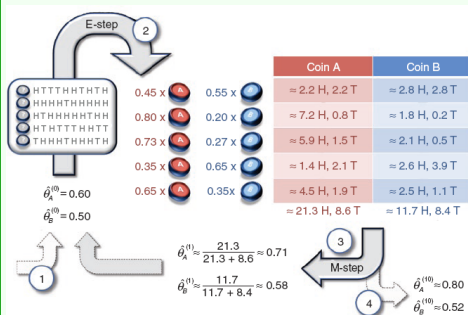
Rather than picking the single most likely completion of the missing coin assignments, EM algorithm refines the completion.

Refinement Cont'd

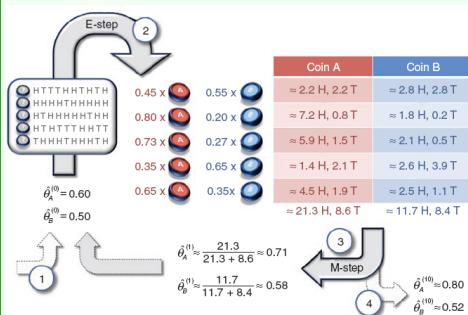


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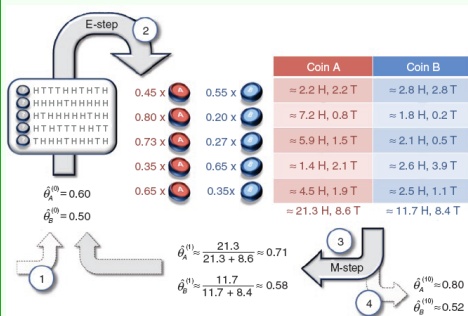


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- These probabilities are used to create a weighted training set;
- Finally, EM algorithm deals with weighted training examples provides new parameter estimates, $\hat{\theta}^{(t+1)}$.

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Filtering and smoothing EM algorithms arise by repeating this two-step procedure:

- **E-step**: Determine the conditional expectation

$$E_{Z|\theta_n}(l(\theta|\mathbf{X}))$$

- **M-step**: Maximize this expression w.r.t. θ .

$$\theta_{n+1} = \operatorname{argmax}_{\theta} E_{Z|\theta_n}(l(\theta|\mathbf{X})).$$

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The log-likelihood function is

$$\log L(\mu_M, \mu_F | y_i) = \sum_{i=1}^n [I_{C_i=M} \log P(y_i|M)P(M) + I_{C_i=F} \log P(y_i|F)P(F)]$$

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Note that $I_{C_i=M}$ is a r.v. Let's look at the $P(C_i = M | y_i)$

$$\begin{aligned} P(C_i = M | y_i) &= \frac{P(y_i | C_i = M)P(C_i = M)}{P(y_i | C_i = M)P(C_i = M) + P(y_i | C_i = F)P(C_i = F)} \\ &= \frac{\pi_M N(y_i | \mu_M, \sigma^2)}{\pi_M N(y_i | \mu_M, \sigma^2) + \pi_F N(y_i | \mu_F, \sigma^2)} \doteq q(M) \end{aligned}$$

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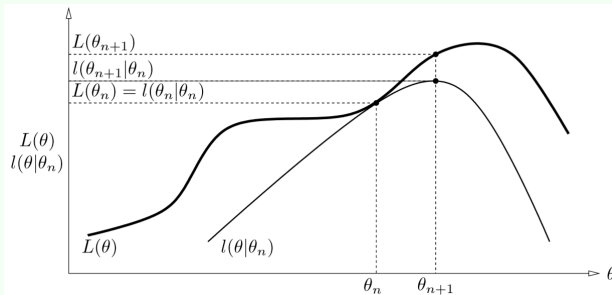
That is,

$$\mu_M^{(k)} = \frac{\sum_{i=1}^n q(M)^{(k)} y_i}{\sum_{i=1}^n q(M)^{(k)}}, \mu_F^{(k)} = \frac{\sum_{i=1}^n (1 - q(F)^{(k)}) y_i}{\sum_{i=1}^n (1 - q(F)^{(k)})}$$

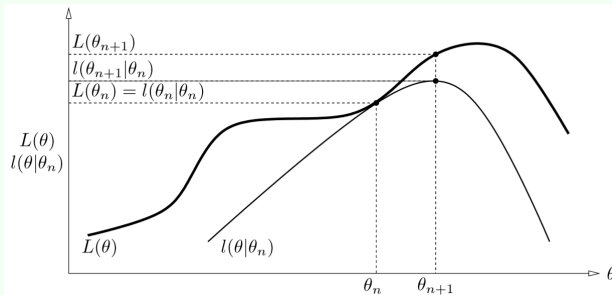
Convergence of EM algorithm

$$\begin{aligned}l(\theta|\mathbf{x}) &= \sum_{i=1}^n \log p(x_i; \theta) = \sum_{i=1}^n \log \sum_z p(x_i, z; \theta) \\&= \sum_{i=1}^n \log \sum_z p(z; \theta_n) \frac{p(x_i, z; \theta)}{p(z; \theta_n)} \\&\geq \sum_{i=1}^n \sum_z p(z; \theta_n) \log \frac{p(x_i, z; \theta)}{p(z; \theta_n)} \\&= \sum_{i=1}^n \sum_z p(z; \theta_n) \log p(x_i, z; \theta) - n \sum_z p(z; \theta_n) \log p(z; \theta_n) \\&= Q(\theta|\theta_n) + H(P(z; \theta_n)) \equiv F(p(z; \theta_n), \theta) \\Q(\theta_{n+1}|\theta_n) &= Q(\theta_n|\theta_n)\end{aligned}$$

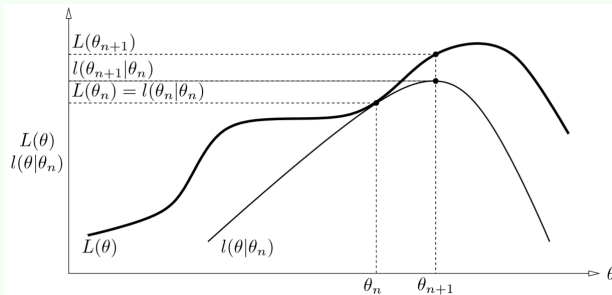
Convergence of EM algorithm Cont'd



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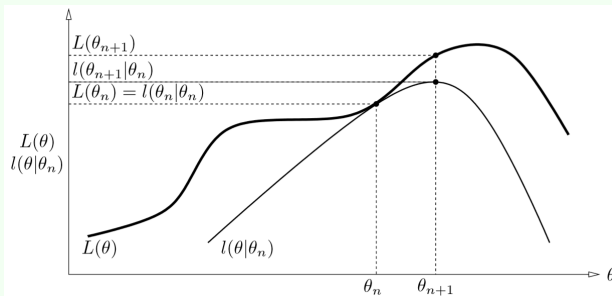


Convergence of EM algorithm Cont'd



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Convergence of EM algorithm Cont'd



- The EM Algorithm always improves a parameter's estimation through this multi-step process;
- However, it sometimes needs a few random starts to find the best model because the algorithm can hone in on a local maxima that is not that close to the (optimal) global maxima.

MLE VS. EM algorithm

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 - Steps 2 through 4 are repeated until stability

Take-home messages

- Motivation
- MLE
- EM Algorithm