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Addendum: The EM Algorithm

In many problems MLE based on observed data X would be greatly simplified if we had additionally observed another piece of data Y.Y is called the hidden or latent data.

**Example 1**  $X \sim \mathcal{N}(H\theta, I)$  can be modeled as:

$$Y_{k \times 1} = \theta + W_1$$
  
$$X_{n \times 1} = H_{n \times k} Y + W_2$$

such that  $HW_1 + W_2 \sim \mathcal{N}(0, I)$ .

If we just have X, then we must solve a system of equations to obtain the MLE. If the dimension is large, then computing the MLE is quite expensive(i.e. the inversion is at least  $O(\max(nk^2, k^3)))$ . But if we also have Y, then the MLE can be computed with O(k) as we know  $\hat{\theta} = Y$ .

## Example 2

$$\begin{aligned} x_i & \stackrel{iid}{\sim} & p\mathcal{N}(\mu_0, \sigma_0^2) + (1-p)\mathcal{N}(\mu_1, \sigma_1^2) \\ y_i & \stackrel{iid}{\sim} & \text{Bernoulli}(p) = p^{1-y_i}(1-p)^{y_i} \\ x_i | y_i = l & \sim & \mathcal{N}(\mu_l, \sigma_l^2) \end{aligned}$$

Given  $\{(x_i, y_i)\}_{i=1}^n$ , we have:

$$\hat{\mu}_{l} = \frac{1}{\sum 1_{y_{i}=l}} \sum_{i:y_{i}=l} x_{i}$$

$$\hat{\sigma}_{l} = \frac{1}{\sum 1_{y_{i}=l}} \sum_{i:y_{i}=l} (x_{i} - \hat{\mu}_{l})^{2}$$

$$\hat{p} = \frac{\sum 1_{y_{i}=l}}{n}$$

MLE's are easy to compute here. However, if we only have  $\{x_i\}_{i=1}^n$ , the computation of MLE is a complicated, non-convex optimization, where we can apply EM algorithm to compute. The application of EM algorithm in this situation is shown in **Example 4**.

## Main Idea

Let  $L(\theta) = \log p(x|\theta)$  and also define the complete data log-like:

$$L_c(\theta) = \log p(x, y|\theta) = \log p(y|x|\theta)p(x|\theta)$$
$$= \log p(y|x|\theta) + \log p(x|\theta) = \log p(y|x|\theta) + L(\theta)$$

Suppose our current guess of  $\theta$  is  $\theta^{(t)}$  and that we would like to imporve this guess. Consider

$$L(\theta) - L(\theta^{(t)}) = L_c(\theta) - L_c(\theta^{(t)}) + \log \frac{p(y|x|\theta^{(t)})}{p(y|x|\theta)}$$

Now take expectation of both sides with respect to  $y \sim p(y|x|\theta^{(t)})$ , we have:

$$L(\theta) - L(\theta^{(t)}) = \mathbb{E}_y[L_c(\theta)] - \mathbb{E}_y[L_c(\theta^{(t)})] + D(p(y|x|\theta^{(t)})||p(y|x|\theta))$$

As  $D(p(y|x|\theta^{(t)})||p(y|x|\theta)) \ge 0$ , we have the following inequality:

$$L(\theta) - L(\theta^{(t)}) \ge \mathbb{E}_y[L_c(\theta)] - \mathbb{E}_y[L_c(\theta^{(t)})] = Q(\theta, \theta^{(t)}) - Q(\theta^{(t)}, \theta^{(t)})$$

Note:  $Q(\theta, \theta') = \mathbb{E}_{p(y|x|\theta')}[\log p(x, y|\theta)]$  is the expectation of complete data log-likelihood. We choose  $\theta^{(t+1)}$  as answer of the following optimization problem:

 $\theta^{(t+1)} = \arg \max_{\theta} Q(\theta, \theta^{(t)})$ 

The relationship between  $\log p(x,\theta)$ ,  $Q(\theta,\theta^{(t)})$ ,  $\theta^t$  and  $\theta^{(t+1)}$  are showed in the following graph:

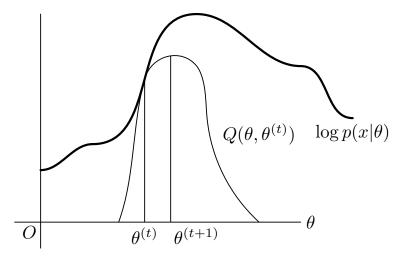


Figure 1: Graphical show of EM algorithm

The process of EM algorithm is as follows: **Init:**  $t = 0, \theta^{(0)} = 0$  or random value Loop:

E step: Compute

$$Q(\theta, \theta^{(t)}) = \mathbb{E}_{p(y|x|\theta^{(t)})}[\log p(x, y|\theta)]$$

M step:

$$\theta^{(t+1)} = \arg \max_{\theta} Q(\theta, \theta^{(t)})$$

End

The E-step and M-step repeat until convergence. **Properties of EM algorithm**:

1.  $\log p(x|\theta^{(0)}) \le \log p(x|\theta^{(1)}) \le \dots$ 

2. It converges to stationary point(e.g. local max)

**Example 3** Original model  $X = H\theta + W$ : Complete model:

$$Y = \theta + W_1 \qquad W_1 \sim \mathcal{N}(0, \alpha^2 I_{k \times k})$$
  
$$X = H_{n \times k} Y + W_2 \qquad W_2 \sim \mathcal{N}(0, I_{n \times n} - \alpha^2 H H^T)$$

Then we construct the complete log-likelihood:

$$\begin{split} \log p(x, y|\theta) &= \log p(x|y|\theta) + \log p(y|\theta) \\ &= constant - \frac{||y - \theta||^2}{2\alpha^2} \\ &= \frac{1}{2\alpha^2} (2\theta^T y - \theta^T \theta - y^T y) + constant \\ &= \frac{1}{2\alpha^2} (2\theta^T y - \theta^T \theta) + constant \end{split}$$

As the part left after taking away the constant is proportional to y, so we only need to calculate  $\mathbb{E}_{p(y|x|\theta^{(t)})}[y]$ . Introduce  $Z_1 = Y$ ,  $Z_2 = X - HY$ , then we have the joint distribution of  $Z_1, Z_2$  as:

$$\begin{bmatrix} Z_1 \\ Z_2 \end{bmatrix} = \mathcal{N}(\begin{bmatrix} \theta \\ 0 \end{bmatrix}, \begin{bmatrix} \alpha^2 I_{k \times k} & 0 \\ 0 & I_{n \times n} - \alpha^2 H H^T \end{bmatrix})$$

$$As \ we \ know \begin{bmatrix} X \\ Y \end{bmatrix} = \begin{bmatrix} H & I_{n \times n} \\ I_{k \times k} & 0 \end{bmatrix} \begin{bmatrix} Z_1 \\ Z_2 \end{bmatrix}, \ we \ know:$$

$$\begin{bmatrix} X \\ Y \end{bmatrix} \sim \mathcal{N}(\begin{bmatrix} H\theta \\ \theta \end{bmatrix}, \begin{bmatrix} I_{n \times n} & \alpha^2 H \\ \alpha^2 H^T & \alpha^2 I_{k \times k} \end{bmatrix})$$

Make a linear transformation, we have:

$$\begin{bmatrix} X \\ Y - \alpha^2 H^T X \end{bmatrix} \sim \mathcal{N}(\begin{bmatrix} H\theta \\ \theta - \alpha^2 H^T H\theta \end{bmatrix}, \begin{bmatrix} I_{n \times n} & 0 \\ 0 & \alpha^2 I_{k \times k} - \alpha^4 H^T H \end{bmatrix})$$

So we have:

$$\mathbb{E}_{p(y|x|\theta^{(t)})}[y] = \alpha^2 H^T x + \theta^{(t)} - \alpha^2 H^T H \theta^{(t)} = y^{(t)}$$

As  $Q(\theta, \theta^{(t)}) = \frac{1}{2\alpha^2} (2\theta^T y^{(t)} - \theta^T \theta) + \text{constant}$ , set  $\frac{\partial Q}{\partial \theta} = 0$ , we have:

 $\theta^{(t+1)} = y^{(t)}$ 

It is easy to calculate the stationary point in this iteration, let  $\theta^{(t+1)} = \theta^{(t)}$ , we have:

$$\theta_{stationary} = (H^T H)^{-1} H^T x$$

which is the answer we are familiar with.

Example 4 Suppose:

$$X_1, X_2, \dots, X_n \stackrel{iid}{\sim} \sum_{j=1}^m p_j \mathcal{N}(\mu_j, \sigma_j^2)$$

We have:

$$p(x, y|\theta) = \prod_{i=1}^{n} \sum_{j=1}^{m} p_j \frac{1}{\sqrt{2\pi\sigma_j}} e^{-\frac{(x_i - \mu_j)^2}{2\sigma_j^2}} \mathbf{1}_{y_i = j}$$

Thus,

$$\log p(x, y | \theta) = \sum_{i=1}^{n} \sum_{j=1}^{m} \log(\frac{p_j}{\sqrt{2\pi\sigma_j}} e^{-\frac{(x_i - \mu_j)^2}{2\sigma_j^2}}) 1_{y_i = j}$$

$$\mathbb{E}_{p(y|x|\theta^{(t)})}[\log p(x,y|\theta)] = \sum_{i=1}^{n} \sum_{j=1}^{m} \log(\frac{p_j}{\sqrt{2\pi\sigma_j}} e^{-\frac{(x_i - \mu_j)^2}{2\sigma_j^2}}) \mathbb{E}_{p(y|x|\theta^{(t)})}[1_{y_i=j}]$$

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$$\begin{split} &= \sum_{i=1}^{n} \sum_{j=1}^{m} \log(\frac{p_{j}}{\sqrt{2\pi\sigma_{j}}} e^{-\frac{(x_{i}-\mu_{j})^{2}}{2\sigma_{j}^{2}}}) \frac{p_{j}^{(t)}\mathcal{N}(x_{i};\mu_{j}^{(t)},(\sigma_{j}^{(t)})^{2})}{\sum_{l=1}^{m} p_{l}^{(t)}\mathcal{N}(x_{i};\mu_{l}^{(t)},(\sigma_{l}^{(t)})^{2})} \\ Denote \ p^{(t)}(y_{i}=j) = \frac{p_{j}^{(t)}\mathcal{N}(x_{i};\mu_{j}^{(t)},(\sigma_{j}^{(t)})^{2})}{\sum_{l=1}^{m} p_{l}^{(t)}\mathcal{N}(x_{i};\mu_{l}^{(t)},(\sigma_{l}^{(t)})^{2})}, \ we \ have \ the \ expression \ of \ Q(\theta, \theta^{(t)}): \\ Q(\theta, \theta^{(t)}) = \sum_{i=1}^{n} \sum_{j=1}^{m} p^{(t)}(y_{i}=j) \log(p_{j}^{(t)}\mathcal{N}(x_{i};\mu_{j},\sigma_{j}^{2})) \\ &= \sum_{i=1}^{n} \sum_{j=1}^{m} p^{(t)}(y_{i}=j) \log(\mathcal{N}(x_{i};\mu_{j},\sigma_{j}^{2})) + \text{constant} \end{split}$$

Set  $\frac{\partial Q}{\partial \theta} = 0$ , we have:

$$\begin{array}{lll} \mu_{j}^{(t+1)} & = & \displaystyle \frac{\sum_{i=1}^{n} p^{(t)}(y_{i}=j)x_{i}}{\sum_{i=1}^{n} p^{(t)}(y_{i}=j)} \\ (\sigma_{j}^{(t+1)})^{2} & = & \displaystyle \frac{\sum_{i=1}^{n} (x_{i}-\mu_{j}^{(t+1)})^{2} p^{(t)}(y_{i}=j)}{\sum_{i=1}^{n} p^{(t)}(y_{i}=j)} \end{array}$$