Lecture 12

Clustering and the EM algorithm

X is a sequence of i.i.d. RV.

$P\{X_i = 0\} = P\{X_i = 1\} = 1/2$

W is also i.i.d given X

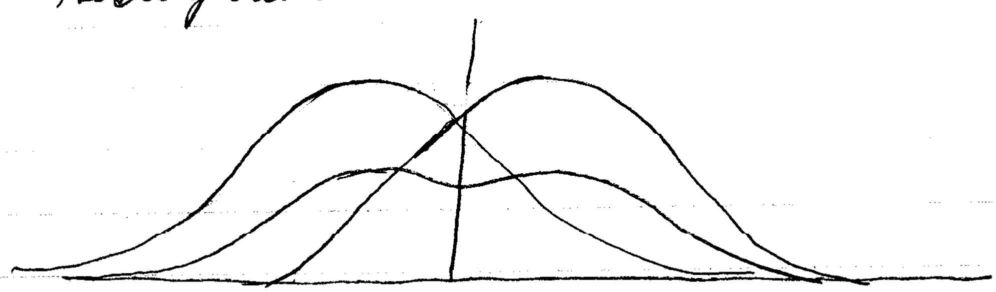
$p(y_i/x_i) \sim N(\mu_{x_i}, \sigma^2_{x_i})$

$(\mu_0, \underset{\gamma_0}{\sigma_0^2})$ – parameters of class 0

$(\mu_1, \underset{\gamma_1}{\sigma_1^2})$ – parameters of class 1.

Question: How do we estimate cluster parameters directly from y?

Histogram



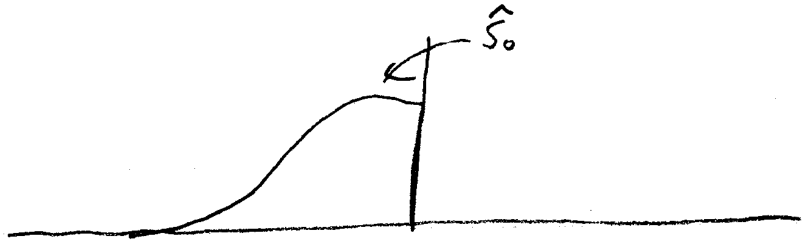
If we know X the problem is easy

$$S_0 = \{i : X_i = 0\}$$
$$S_1 = \{i : X_i = 1\}$$

$$\hat{\mu}_0 = \frac{1}{|S_0|} \sum_{i \in S_0} y_i \qquad \hat{\sigma}_0^2 = \frac{1}{|S_0|} \sum_{i \in S_0} (y_i - \hat{\mu}_0)^2$$

What if we estimate S_0?

$$\hat{S}_0 = \{ i : Y_i \le 0 \}$$



$$\frac{1}{|\hat{S}_0|} \sum_{i \in \hat{S}_0} y_i < \frac{1}{|S_0|} \sum_{i \in S_0} y_i$$

This is called the "incomplete data" problem because we are missing X.

$$\hat{\theta}_{ML} = \arg\max_{\theta} p(y|\theta)$$

$$= \arg\max_{\theta} \left\{ \int p(y|x,\theta)\, p(x|\theta)\, dx \right\}$$

difficult to do

New approach:

$$\log p(y|\theta') = \int \log p(y|\theta')\, p(x|y,\theta)\, dx$$

$p(y,x|\theta') = p(x|y\theta')p(y|\theta$

$$= \int \log \left\{ \frac{p(y,x|\theta')}{p(x|y,\theta')} \right\} p(x|y,\theta)\, dx$$

$$= \int \log p(y,x|\theta')\, p(x|y,\theta)\, dx$$

$$- \int \log p(x|y,\theta')\, p(x|y,\theta)\, dx$$

Define

$$Q(\theta',\theta) = \int \log p(y,x|\theta')\, p(x|y,\theta)\, dx$$

$$H(\theta',\theta) = -\int \log p(x|y,\theta')\, p(x|y,\theta)\, dx$$

$$\log p(y|\theta') = Q(\theta',\theta) + H(\theta',\theta)$$

<u>Theorem</u> $\forall \theta$

$$\theta = \arg\min_{\theta'} H(\theta', \theta)$$

<u>proof</u>

W.L.O.G. use $p(x|\theta)$ in place of $p(x|y,\theta)$

$$0 = \log\left\{\int p(x|\theta')\,dx\right\}$$

$$= \log\left\{\int \frac{p(x|\theta')}{p(x|\theta)}\,p(x|\theta)\,dx\right\}$$

(Jensen's inequality)

$$\geq \int \log\left\{\frac{p(x|\theta')}{p(x|\theta)}\right\} p(x|\theta)\,dx$$

$$= \int \log p(x|\theta')\,p(x|\theta)\,dx$$

$$- \int \log p(x|\theta)\,p(x|\theta)\,dx$$

$$0 \geq -H(\theta', \theta) + H(\theta, \theta)$$

$$H(\theta', \theta) \geq H(\theta, \theta)$$

Intuition

$$\theta = \arg\min_{\theta'} H(\theta', \theta)$$

$$= \arg\min_{\theta'} -\int \log p(x \mid \theta')\, p(x \mid \theta)\, dx$$

$$= \arg\min_{\theta'} -E_\theta \left[\log p(X \mid \theta') \right]$$

$$= \arg\max_{\theta'} \left\{ \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} \log p(X_i \mid \theta') \right\}$$

where X_i are i.i.d. r.v's with distribution $p(x \mid \theta)$

$$= \lim_{N \to \infty} \arg\min_{\theta'} \left\{ \log p(x_1, \ldots x_N \mid \theta') \right\}$$

$\Rightarrow$ ML estimate of θ is consistant

Theorem $Q(\theta', \theta) > Q(\theta, \theta) \Rightarrow p(y|\theta') > p(y|\theta)$

proof

$$\log p(y|\theta') = Q(\theta', \theta) + H(\theta', \theta)$$

$$> Q(\theta, \theta) + H(\theta', \theta)$$

$$\geq Q(\theta, \theta) + H(\theta, \theta)$$

$$= \log p(y|\theta)$$

New Algorithm:

Expectation Maximization (EM)

Baum Welch

$$\theta^{(k+1)} = \underset{\theta}{\operatorname{argmax}}\ Q(\theta, \theta^{(k)})$$

$$= \underset{\theta}{\operatorname{argmax}} \int \log p(y, x|\theta)\, p(x|y, \theta^{(k)})\, dx$$

maximization expectation

Example

$\{X_i\}_{i=1}^{N}$ i.i.d with $P\{X_i=0\} = P\{X_i=1\} = 1/2$

$\{Y_i\}_{i=1}^{N}$ conditionally i.i.d. with

$$p(y_i | x_i) \sim N(\mu_{x_i}, \underset{\gamma_{x_i}}{\overset{\|}{\sigma_{x_i}^2}})$$

$$\gamma_0 = (\mu_0, \gamma_0) \rightarrow \text{class } 0$$
$$\gamma_1 = (\mu_1, \gamma_1) \rightarrow \text{class } 1$$

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

not a function of θ.

$$\log p(y\,x|\theta) = \sum_{i=1}^{N} \log p(y_i | \psi_0)\,\delta(x_i) + \sum_{i=1}^{N} \log p(y_i | \psi_1)\,\delta(x_i - 1) - N \log 2$$

$$Q(\theta', \theta) = \int \log p(y, x|\theta')\, p(x|y, \theta)\, dx$$

$$= E\left[\log p(Y, X | \theta') \,/\, Y = y, \theta \right]$$

$$= \sum_{i=1}^{N} \log p(y_i | \psi_0)\, E\left[\delta(x_i) \,/\, Y = y, \theta \right] + \sum_{i=1}^{N} \log p(y_i | \psi_1)\, E\left[\delta(x_i - 1) \,/\, Y = y, \theta \right] - N \log 2$$

$$E[\delta(X_i) | Y = y, \theta] = P\{ X_i = 0 \,/\, Y = y, \theta \} = p(x_i = 0 / y, \theta)$$

$$p(x_i | y, \theta) = \frac{p(y_i | x_i, \theta)\, p(x_i)}{\sum_{\tilde{x}_i} p(y_i | \tilde{x}_i, \theta)\, p(\tilde{x}_i)}$$

easy to compute

(E-step) $\triangleq f(x_i | y_i, \theta)$

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Since

$$\log p(y_i \mid \varphi) = -\frac{1}{2\sigma^2}(y_i-\mu)^2 - \frac{1}{2}\log(2\pi\sigma^2)$$

$$Q(\theta',\theta) = \sum_{i=1}^{N}\left\{-\frac{1}{2\sigma_0^2}(y_i-\mu_0')^2 - \frac{1}{2}\log(2\pi\gamma_0')\right\} f(0 \mid y_i\,\theta)$$

$$+\sum_{i=1}^{N}\left\{-\frac{1}{2\sigma_1^2}(y_i-\mu_1')^2 - \frac{1}{2}\log(2\pi\gamma_1')\right\} f(1 \mid y_i\,\theta)$$

$$-N\log 2$$

1^{st} term only a function of (μ_0, σ_0^2)
2^{nd} term only a function of (μ_1, σ_1^2)

$$\hat{\theta} = \underset{\theta'}{\arg\max}\; Q(\theta',\theta)$$

Answer:

$$\hat{N}_0 = \sum_{i=1}^{N} f(0 \mid y_i,\theta)$$ → average ~~#~~ of 0 points

$$\hat{\mu}_0 = \frac{1}{\hat{N}_0}\sum_{i=1}^{N} y_i f(0 \mid y_i,\theta)$$ → weighted mean

$$\hat{\gamma}_0 = \frac{1}{\hat{N}_0}\sum_{i=1}^{N}(y_i-\hat{\mu}_0)^2 f(0 \mid y_i,\theta)$$
→ weighted variance

$$\hat{N}_1 = \sum_{i=1}^{N} f(1/y_i, \theta)$$

$$\hat{\mu}_1 = \frac{1}{\hat{N}_1} \sum_{i=1}^{N} y_i \, f(1/y_i \, \theta)$$

$$\hat{\gamma}_1 = \frac{1}{\hat{N}_1} \sum_{i=1}^{N} (y_i - \hat{\mu}_1)^2 \, f(1/y_i \, \theta)$$

Repeat this procedure until
you converge!

Convergence of EM algorithm

Assume

1) The ML estimate of $p(y|\theta)$ exists

2) $Q(\theta', \theta)$ and $H(\theta', \theta)$ are well defined, continuous and differentiable functions of θ, and θ'

3) θ finite dimensional

Theorem If $\theta^* = \lim_{K \to \infty} \theta^{(K)}$ exists,

then $\nabla_\theta p(y|\theta) \Big|_{\theta = \theta^*} = 0$

proof

1) $\nabla_\theta Q(\theta ; \theta^*) \Big|_{\theta = \theta^*} = 0$

steady state condition

2) $\nabla_\theta H(\theta, \theta^*) \Big|_{\theta = \theta^*} = 0$

result of theorem

3) $\nabla_\theta \log p(y|\theta) \Big|_{\theta = \theta^*}$

$= \nabla_\theta Q(\theta, \theta^*) \Big|_{\theta = \theta^*} + \nabla_\theta H(\theta^*, \theta) \Big|_{\theta = \theta^*}$

$= 0 + 0 = 0$

Theorem If $p(y|\theta)$ is a strictly concave function of θ then

$$\theta^* = \lim_{k\to\infty} \theta^{(k)} = \theta_{ML}$$

proof

1) $\lim_{k\to\infty} \theta^{(k)}$ exists

2) $\nabla_\theta \, p(y|\theta)\big|_{\theta=\theta^*} = 0$

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Example

As before, but

$$\left.\begin{array}{l}(\mu_0, \sigma_0^2)\\(\mu_1, \sigma_1^2)\end{array}\right\} \text{ are known}$$

$$P\{X_i = 0\} = \pi_0 \qquad P\{X_i = 1\} = 1 - \pi_0$$

$p(y_i | x_i)$ known $\quad \theta = \pi_0$

$$p(y|\theta) = \prod_{i=1}^{N} \Big(\theta p(y|0) + (1-\theta) p(y|1) \Big)$$

$$\log p(y|\theta) = \sum_{i=1}^{N} \log \Big(\theta p(y|0) + (1-\theta) p(y|1) \Big)$$

$\log p(y|\theta)$ is a convex function of θ.

$\Rightarrow$ EM algorithm converges to θ_{ML}

$$\log p(y, x|\theta) = \underbrace{\log p(y|x, \theta)}_{\text{does not depend on } \theta} + \log p(x|\theta)$$

Let $K = \# x_i = 0 = \sum_{i=1}^{N} \delta(x_i)$

$$\log p(x|\theta) = \log \Big(\theta^K (1-\theta)^{N-K} \Big)$$

$$\log p(x|\theta) = K \log\theta + (N-K)\log(1-\theta)$$

$$= K(\log\theta - \log(1-\theta)) + N\log(1-\theta)$$

$$Q(\theta',\theta) = \int \log p(y,x|\theta')\, p(x|y,\theta)\, dx$$

$$= E\left[K(\log\theta' - \log(1-\theta')) + C \,/\, Y=y,\theta\right]$$

$$= E[K \,/\, Y=y,\theta]\,(\log\theta' - \log(1-\theta'))$$

$$E[K \,/\, Y=y,\theta] = E\left[\sum_{i=1}^{N}\delta(X_i) \,/\, Y=y,\theta\right]$$

$$= \sum_{i=1}^{N} E[\delta(X_i) \,/\, Y=y,\theta]$$

$$= \sum_{i=1}^{N} P\{X_i=0 \,/\, Y_i=y_i,\theta\}$$

$$= \sum_{i=1}^{N}\left\{\frac{p(y_i|X_i=0)\,\theta}{p(y_i|X_i=0)\theta + p(y_i|X_i=1)(1-\theta)}\right. \Rightarrow \text{easy to compute}$$

$$= \bar{K} \leftarrow \text{expected number of } x_i\text{'s} = 0 \text{ given } y \text{ and } \theta$$

argmax

$$\arg\max_{\theta'} Q(\theta', \theta)$$

$$= \arg\max_{\theta'} \bar{K} \left(\log \theta' - \log(1-\theta') \right)$$

$$= \frac{\bar{K}}{N} \leftarrow \text{same as 1}^{st} \text{ homework}$$

<u>EM algorithm</u>

$$\theta^{(k+1)} = \frac{1}{N} \sum_{i=1}^{N} \left\{ \frac{p(y_i \mid x_i = 0)\,\theta}{p(y_i \mid x_i = 0)\,\theta + p(y_i \mid x_i = 1)(1-\theta)} \right\}$$

<u>Exercise</u>

Derive EM algorithm when

$$p(y_i \mid x_i) \sim N(\mu_{x_i}, \sigma_{x_i}^2)$$

$$P\{x_i = 0\} = \pi_0 \quad P\{x_i = 1\} = 1 - \pi_0$$

$$\theta = (\pi_0, \mu_0, \sigma_0^2, \mu_1, \sigma_1^2)$$