

Principles of Parameter Estimation

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PRELIMINARIES

Given: a set of observations $\mathcal{D} = \{x_i\}_{i=1}^n$, $x_i \in \mathcal{X}$

Objective: find a model $\hat{f} \in \mathcal{F}$ that models the phenomenon well

Requirements:

- (i) the ability to generalize well
- (ii) the ability to incorporate prior knowledge and assumptions
- (iii) scalability

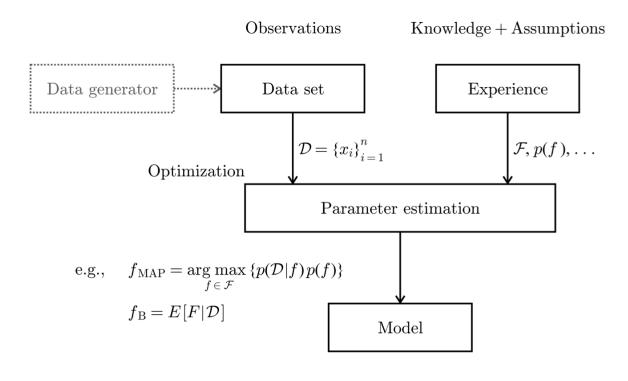
Terminology through an example: $\mathcal{D} = \{3.1, 2.4, -1.1, 0.1\}$

What is the data generator?

$$\mathcal{F} = \text{Gaussian}(\mu, \sigma^2), \, \mu \in \mathbb{R}, \, \sigma \in \mathbb{R}^+$$

Parameter estimation

STATISTICAL FRAMEWORK



MAXIMUM A POSTERIORI INFERENCE

Idea:

$$f_{\text{MAP}} = \underset{f \in \mathcal{F}}{\operatorname{arg max}} \{ p(f|\mathcal{D}) \},$$

where $p(f|\mathcal{D})$ is called the posterior distribution.

How do we calculate it?

$$p(f|\mathcal{D}) = \frac{p(\mathcal{D}|f) \cdot p(f)}{p(\mathcal{D})}$$

where $p(\mathcal{D}|f) = \text{likelihood}$, p(f) = prior, and $p(\mathcal{D}) = \text{data distribution}$.

MAXIMUM A POSTERIORI INFERENCE

Finding the data distribution:

$$p(\mathcal{D}) = \begin{cases} \sum_{f \in \mathcal{F}} p(\mathcal{D}|f) p(f) & f : \text{discrete} \\ \\ \int_{\mathcal{F}} p(\mathcal{D}|f) p(f) df & f : \text{continuous} \end{cases}$$

We can now simplify the process if we observe that

$$p(f|\mathcal{D}) = \frac{p(\mathcal{D}|f) \cdot p(f)}{p(\mathcal{D})}$$
$$\propto p(\mathcal{D}|f) \cdot p(f)$$

MAXIMUM LIKELIHOOD INFERENCE

Express the posterior distribution as

$$p(f|\mathcal{D}) = \frac{p(\mathcal{D}|f) \cdot p(f)}{p(\mathcal{D})}$$
$$\propto p(\mathcal{D}|f) \cdot p(f)$$

Now, ignore p(f) to get

$$f_{\mathrm{ML}} = \underset{f \in \mathcal{F}}{\operatorname{arg\,max}} \{ p(\mathcal{D}|f) \}$$

There are technical problems with this approach.

Examples of Maximum Likelihood Inference

Example: $\mathcal{D} = \{2, 5, 9, 5, 4, 8\}$ is an i.i.d. sample from $Poisson(\lambda), \lambda \in \mathbb{R}^+$

Find λ

Solution: Poisson probability mass function is $p(x|\lambda) = \frac{\lambda^x e^{-\lambda}}{x!}$

$$\lambda_{\mathrm{ML}} = \underset{\lambda \in (0,\infty)}{\mathrm{arg\,max}} \left\{ p(\mathcal{D}|\lambda) \right\}.$$

Likelihood:
$$p(\mathcal{D}|\lambda) = p(\{x_i\}_{i=1}^n | \lambda)$$

$$= \prod_{i=1}^n p(x_i | \lambda)$$

$$= \frac{\lambda^{\sum_{i=1}^n x_i} \cdot e^{-n\lambda}}{\prod_{i=1}^n x_i!}.$$

Examples of Maximum Likelihood Inference

Likelihood:
$$p(\mathcal{D}|\lambda) = \frac{\lambda^{\sum_{i=1}^{n} x_i} \cdot e^{-n\lambda}}{\prod_{i=1}^{n} x_i!}$$

Log-likelihood:
$$ll(\mathcal{D}, \lambda) = \ln \lambda \sum_{i=1}^{n} x_i - n\lambda - \sum_{i=1}^{n} \ln (x_i!)$$

Optimization:

Solution:

$$\frac{\partial ll(\mathcal{D}, \lambda)}{\partial \lambda} = \frac{1}{\lambda} \sum_{i=1}^{n} x_i - n$$
$$= 0$$

$$\lambda_{\text{ML}} = \frac{1}{n} \sum_{i=1}^{n} x_i$$
$$= 5.5$$

MAP and ML estimates are called the point estimates.

EXAMPLES OF MAP INFERENCE

Example: $\mathcal{D} = \{2, 5, 9, 5, 4, 8\}$ is i.i.d. sample from $Poisson(\lambda), \lambda \in \mathbb{R}^+$

Assume λ is taken from $\Gamma(x|k,\theta)$ with parameters k=3 and $\theta=1$

Find λ

Solution: Poisson: $p(x|\lambda) = \frac{\lambda^x e^{-\lambda}}{x!}$

Gamma: $\Gamma(x|k,\theta) = \frac{x^{k-1}e^{-\frac{x}{\theta}}}{\theta^k\Gamma(k)}$, where x > 0, k > 0, and $\theta > 0$.

Likelihood: $p(\mathcal{D}|\lambda) = \frac{\lambda^{\sum_{i=1}^{n} x_i} \cdot e^{-n\lambda}}{\prod_{i=1}^{n} x_i!}$

Prior: $p(\lambda) = \frac{\lambda^{k-1} e^{-\frac{\lambda}{\theta}}}{\theta^k \Gamma(k)}$

EXAMPLES OF MAP INFERENCE

Log-likelihood:

$$\ln p(\lambda|\mathcal{D}) \propto \ln p(\mathcal{D}|\lambda) + \ln p(\lambda)$$

$$= \ln \lambda(k - 1 + \sum_{i=1}^{n} x_i) - \lambda(n + \frac{1}{\theta}) - \sum_{i=1}^{n} \ln x_i! - k \ln \theta - \ln \Gamma(k)$$

We now obtain

$$\lambda_{\text{MAP}} = \frac{k - 1 + \sum_{i=1}^{n} x_i}{n + \frac{1}{\theta}}$$
$$= 5$$

ANOTHER EXAMPLE

Example: $\mathcal{D} = \{x_i\}_{i=1}^n$ is i.i.d. sample from Gaussian (μ, σ^2)

Find μ and σ

Solution: Gaussian: $p(x|\mu,\sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$

$$\mu_{\text{ML}} = \frac{1}{n} \sum_{i=1}^{n} x_i$$

$$\sigma_{\text{ML}}^2 = \frac{1}{n} \sum_{i=1}^{n} (x_i - \mu_{\text{ML}})^2.$$

RELATIONSHIP TO KULLBACK-LEIBLER (KL) DIVERGENCE

The KL divergence between two probability distributions p(x) and q(x) is

$$D_{\mathrm{KL}}(p||q) = \int_{-\infty}^{\infty} p(x) \log \frac{p(x)}{q(x)} dx$$

Assume now the data is generated according to some $p(x|\theta_t)$. We estimated it as $p(x|\theta)$.

Let's look at the KL divergence

$$D_{\mathrm{KL}}(p(x|\theta_t)||p(x|\theta)) = \int_{-\infty}^{\infty} p(x|\theta_t) \log \frac{p(x|\theta_t)}{p(x|\theta)} dx - E\left[\log p(x|\theta)\right]$$
$$= \int_{-\infty}^{\infty} p(x|\theta_t) \log \frac{1}{p(x|\theta)} dx - \int_{-\infty}^{\infty} p(x|\theta_t) \log \frac{1}{p(x|\theta_t)} dx.$$

RELATIONSHIP TO KULLBACK-LEIBLER (KL) DIVERGENCE

$$\frac{1}{n} \sum_{i=1}^{n} \log p(x_i | \theta) \quad \stackrel{a.s.}{\to} \quad E[\log p(x | \theta)]$$

when $n \to \infty$.

Conclusion:

When $n \to \infty$, ML estimation implies $p(x|\theta_{\text{ML}}) = p(x|\theta_t)$

This usually implies $\theta_{\rm ML} = \theta_t$

PARAMETER ESTIMATION FOR MIXTURES OF DISTRIBUTIONS

Given: a set of observations $\mathcal{D} = \{x_i\}_{i=1}^n$, $x_i \in \mathcal{X}$

$$p(x|\theta) = \sum_{j=1}^{m} w_j p(x|\theta_j).$$
 $w_j \ge 0, \quad \sum_{j=1}^{m} w_j = 1.$

where $\theta = (w_1, w_2, \dots, w_m, \theta_1, \theta_2, \dots, \theta_m)$

Example: Consider a mixture of m=2 exponential distributions.

$$p(x|\theta_i) = \lambda_i e^{-\lambda_j x}$$
, where $\lambda_i > 0$

$$p(x|\lambda_1, \lambda_2, w_1, w_2) = w_1 \cdot \lambda_1 e^{-\lambda_1 x} + w_2 \cdot \lambda_2 e^{-\lambda_2 x}$$

where $\lambda_1, \lambda_2 > 0, w_1, w_2 \ge 0, \text{ and } w_1 = 1 - w_2$

PARAMETER ESTIMATION FOR MIXTURES OF DISTRIBUTIONS

Likelihood:

$$p(\mathcal{D}|\theta) = \prod_{i=1}^{n} p(x_i|\theta)$$
$$= \prod_{i=1}^{n} \left(\sum_{j=1}^{m} w_j p(x_i|\theta_j) \right)$$

 $p(\mathcal{D}|\theta)$ has $O(m^n)$ terms. It can be calculated in O(mn) time as a log-likelihood.

How can we find θ ? Is there a closed-form solution?

Suppose we know what data point is generated by what mixing component.

That is, $\mathcal{D}_{xy} = \{(x_i, y_i)\}_{i=1}^n$ is an i.i.d. sample from some distribution p(x, y), where $y \in \mathcal{Y} = \{1, 2, ..., m\}$ specifies the mixing component.

$$p(\mathcal{D}_{xy}|\theta) = \prod_{i=1}^{n} p(x_i, y_i|\theta)$$
$$= \prod_{i=1}^{n} p(x_i|y_i, \theta)p(y_i|\theta)$$
$$= \prod_{i=1}^{n} w_{y_i}p(x_i|\theta_{y_i}),$$

where $w_j = P(y = j)$.

Log-likelihood:

$$\log p(\mathcal{D}_{xy}|\theta) = \sum_{i=1}^{n} (\log w_{y_i} + \log p(x_i|\theta_{y_i}))$$
$$= \sum_{j=1}^{m} n_j \log w_j + \sum_{i=1}^{n} \log p(x_i|\theta_{y_i}),$$

where n_j is the number of data points in \mathcal{D}_{xy} generatedy the j-th mixing component.

Constrained optimization: Let's first find w

$$L(\mathbf{w}, \alpha) = \sum_{j=1}^{m} n_j \log w_j + \alpha \left(\sum_{j=1}^{m} w_j - 1 \right)$$

where α is the Lagrange multiplier.

Set $\frac{\partial}{\partial w_k} L(\mathbf{w}, \alpha) = 0$ for every $k \in \mathcal{Y}$ and $\frac{\partial}{\partial \alpha} L(\mathbf{w}, \alpha) = 0$. Solve it.

It follows that $w_k = -\frac{n_k}{\alpha}$ and $\alpha = -n$.

$$w_k = \frac{1}{n} \sum_{i=1}^n I(y_i = k),$$

where $I(\cdot)$ is the indicator function.

To find all θ_j , we need to get concrete.

$$\frac{\partial}{\partial \lambda_k} \sum_{i=1}^n \log p(x_i | \lambda_{y_i}) = 0,$$

for each $k \in \mathcal{Y}$.

We obtain that

$$\lambda_k = \frac{n_k}{\sum_{i=1}^n I(y_i = k) \cdot x_i},$$

for each $k \in \mathcal{Y}$.

Recall that

$$w_k = \frac{1}{n} \sum_{i=1}^n I(y_i = k)$$

If the mixing component designations y are known, the parameter estimation is greatly simplified.

Suppose we know the θ but not the mixing componen designations..

Looks like clustering, right? Let's see. Express

see. Express
$$p(\mathbf{y}|\mathcal{D}, \theta) = \prod_{i=1}^{n} p(y_i|x_i, \theta)$$
$$= \prod_{i=1}^{n} \frac{w_{y_i} p(x_i|\theta_{y_i})}{\sum_{j=1}^{m} w_j p(x_i|\theta_j)}$$

and subsequently find the best configuration out of m^n possibilities.

Data is i.i.d. so y_i can be estimated separately. The MAP estimate for y_i

$$\hat{y}_i = \underset{k \in \mathcal{Y}}{\operatorname{arg max}} \left\{ p(y_i | x_i, \theta) \right\} \qquad \qquad p(y_i | x_i, \theta) = \frac{w_{y_i} p(x_i | \theta_{y_i})}{\sum_{j=1}^m w_j p(x_i | \theta_j)}$$

CLASSIFICATION EXPECTATION MAXIMIZATION (CEM)

- 1. Initialize $\lambda_k^{(0)}$ and $w_k^{(0)}$ for $\forall k \in \mathcal{Y}$
- 2. Set t = 0
- 3. Repeat until convergence

(a)
$$\hat{y}_i^{(t)} = \underset{k \in \mathcal{Y}}{\arg \max} \left\{ p\left(y_i = k | x_i, \boldsymbol{w}^{(t)}, \boldsymbol{\lambda}^{(t)}\right) \right\}$$

for $\forall i \in \{1, 2, \dots, n\}$

(b)
$$w_k^{(t+1)} = \frac{1}{n} \sum_{i=1}^n I(\hat{y}_i^{(t)} = k)$$

(c)
$$\lambda_k^{(t+1)} = \frac{\sum_{i=1}^n I(\hat{y}_i^{(t)} = k)}{\sum_{i=1}^n I(\hat{y}_i^{(t)} = k) \cdot x_i}$$

- (d) t = t + 1
- 4. Report $\lambda_k^{(t)}$ and $w_k^{(t)}$ for $\forall k \in \mathcal{Y}$

Contains all w_k Contains all λ_k (a) $\hat{y}_i^{(t)} = \underset{k \in \mathcal{Y}}{\operatorname{arg max}} \left\{ p\left(y_i = k | x_i, \boldsymbol{w}^{(t)}, \boldsymbol{\lambda}^{(t)}\right) \right\} \qquad p(y_i = k | x_i, \boldsymbol{w}, \boldsymbol{\lambda}) = \frac{p(y_i = k | w_k) \cdot p(x_i | \lambda_k)}{\sum_{i=1}^m p(y_i = j | w_i) \cdot p(x_i | \lambda_i)}$ $= \frac{w_k p(x_i|\lambda_k)}{\sum_{i=1}^m w_i p(x_i|\lambda_i)}$

EXPECTATION MAXIMIZATION

EM

1. Initialize $\lambda_k^{(0)}$ and $w_k^{(0)}$ for $\forall k \in \mathcal{Y}$

- 2. Set t = 0
- 3. Repeat until convergence

(a)
$$r_{ik}^{(t)} = p(y_i = k | x_i, \boldsymbol{w}^{(t)}, \boldsymbol{\lambda}^{(t)})$$

for $\forall i \in \{1, 2, \dots, n\}$ and $\forall k \in \mathcal{Y}$

(b)
$$w_k^{(t+1)} = \frac{1}{n} \sum_{i=1}^n r_{ik}^{(t)}$$

(c)
$$\lambda_k^{(t+1)} = \frac{\sum_{i=1}^n r_{ik}^{(t)}}{\sum_{i=1}^n r_{ik}^{(t)} \cdot x_i}$$

- (d) t = t + 1
- 4. Report $\lambda_k^{(t)}$ and $w_k^{(t)}$ for $\forall k \in \mathcal{Y}$

CEM

- 1. Initialize $\lambda_k^{(0)}$ and $w_k^{(0)}$ for $\forall k \in \mathcal{Y}$
- 2. Set t = 0
- 3. Repeat until convergence

(a)
$$\hat{y}_i^{(t)} = \underset{k \in \mathcal{Y}}{\operatorname{arg max}} \{ p(y_i = k | x_i, \boldsymbol{w}^{(t)}, \boldsymbol{\lambda}^{(t)}) \}$$

for $\forall i \in \{1, 2, \dots, n\}$

(b)
$$w_k^{(t+1)} = \frac{1}{n} \sum_{i=1}^n I(\hat{y}_i^{(t)} = k)$$

(c)
$$\lambda_k^{(t+1)} = \frac{\sum_{i=1}^n I(\hat{y}_i^{(t)} = k)}{\sum_{i=1}^n I(\hat{y}_i^{(t)} = k) \cdot x_i}$$

- (d) t = t + 1
- 4. Report $\lambda_k^{(t)}$ and $w_k^{(t)}$ for $\forall k \in \mathcal{Y}$

$$p(y_i = k | x_i, \boldsymbol{w}, \boldsymbol{\lambda}) = \frac{w_k p(x_i | \lambda_k)}{\sum_{j=1}^m w_j p(x_i | \lambda_j)}$$

EM APPROACH

Observable data

$$\mathcal{D}_x = \{x_i\}_{i=1}^n.$$

Goal: maximize $ll(\mathcal{D}_x, \theta)$

Partially observable data

$$\mathcal{D}_{xy} = \{(x_i, y_i)\}_{i=1}^n$$

Consider complete data log-likelihood $ll(\mathcal{D}_{xy}, \theta)$

Current Estimate

 $\theta^{(t)}$

E-Step

$$Q(\theta|\theta^{(t)}) = \mathbb{E}_{\boldsymbol{y}}[ll(D_{xy},\theta)|\mathcal{D}_x,\theta^{(t)}]$$

Expectation is taken over the distribution of random vector \boldsymbol{y} (containing y_i as entries) given the observable data \mathcal{D}_x and the current estimate $\theta^{(t)}$.

M-Step

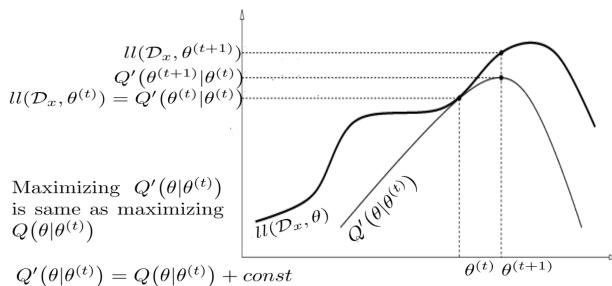
$$\theta^{(t+1)} = \underset{\theta}{\operatorname{arg\,max}} Q(\theta|\theta^{(t)})$$

EM framework is much more general and has many applications beyond mixture models. Hidden markov models, handling missing data, correcting sample selection bias to name a few.

EM Convergence

Converegce follows because the inequality below is true for all θ . Finding a θ that increases the Q function from $Q(\theta^{(t)}|\theta^{(t)})$ makes the RHS positive which ensures that the LHS is also positive and consequently that θ also increases the log-likehood from $ll(\mathcal{D}_x, \theta^{(t)})$.

$$ll(\mathcal{D}_x, \theta) - ll(\mathcal{D}_x, \theta^{(t)}) \ge Q(\theta|\theta^{(t)}) - Q(\theta^{(t)}|\theta^{(t)})$$



Graphical interpretation of a single iteration of the EM: The function $Q'(\theta|\theta^{(t)})$ is upper-bounded by $ll(\mathcal{D}_x, \theta)$. The functions are equal at $\theta = \theta^{(t)}$. The EM algorithm chooses $\theta^{(t+1)}$ as the value of θ for which $Q'(\theta|\theta^{(t)})$ is maximum. Since $ll(\mathcal{D}_{xy}, \theta)$ $Q'(\theta|\theta^{(t)})$ increasing $Q'(\theta|\theta^{(t)})$ ensures that the value of the likelihood function θ $ll(\mathcal{D}_{xy}, \theta)$ is increased at each step.

EM Convergence (proof)

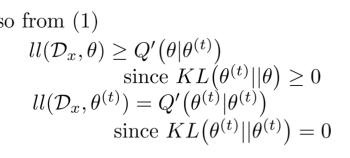
$$ll(\mathcal{D}_{x},\theta) = \log p(\mathcal{D}_{x}|\theta) \qquad \text{Note } KL(\theta^{(t)}||\theta^{(t)}) = 0$$

$$= \log \frac{p(\mathcal{D}_{x}, \mathbf{y}|\theta)}{p(\mathbf{y}|\mathcal{D}_{x}, \theta)} \qquad \text{Thus, from (1)}$$

$$= \log p(\mathcal{D}_{xy}|\theta) - \log p(\mathbf{y}|\mathcal{D}_{x}, \theta) \qquad + KL(\theta^{(t)}||\theta) \qquad + KL(\theta^{(t)}||\theta$$

 $H(\theta^{(t)})$ is short The entropy of the KL divergence begin $p(\boldsymbol{y}|\mathcal{D}_x, \theta^{(t)})$ given by tween $p(\boldsymbol{y}|\mathcal{D}_x, \theta^{(t)})$ and $\mathbb{E}_{\boldsymbol{y}} \left[-\log p(\boldsymbol{y}|\mathcal{D}_x, \theta^{(t)}) \middle| \mathcal{D}_x, \theta^{(t)} \right]$ $p(\boldsymbol{y}|\mathcal{D}_x, \theta)$

 $KL(\theta^{(t)}||\theta)$ is short for



EM FOR EXPONENTIAL MIXTURE

$$ll(\mathcal{D}_{xy}, \theta) = \sum_{i=1}^{n} \log \{ w_{y_i} p(x_i | \lambda_{y_i}) \}$$

$$= \sum_{i=1}^{n} \log \left\{ \prod_{j=1}^{m} (w_j p(x_i | \lambda_j))^{I(y_i = j)} \right\}$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{m} I(y_i = j) (\log w_j + \log p(x_i | \lambda_j))$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{m} I(y_i = j) (\log w_j + \log \lambda_j - \lambda_j x_i)$$

For exponential distribution

$$p(x|\lambda_j) = \lambda_j e^{\lambda_j x}$$

EM FOR EXPONENTIAL MIXTURE: E-STEP

$$Q\Big(\theta|\theta^{(t)}\Big) = \mathbb{E}_{\boldsymbol{y}} \left[ll(D_{xy}, \theta) | \mathcal{D}_{x}, \theta^{(t)} \right]$$

$$= \mathbb{E}_{\boldsymbol{y}} \left[\sum_{i=1}^{n} \sum_{j=1}^{m} I(y_{i} = j) (\log w_{j} + \log \lambda_{j} - \lambda_{j} x_{i}) \middle| \mathcal{D}_{x}, \theta^{(t)} \right]$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{m} \mathbb{E}_{\boldsymbol{y}} \left[I(y_{i} = j) \middle| \mathcal{D}_{x}, \theta^{(t)} \right] (\log w_{j} + \log \lambda_{j} - \lambda_{j} x_{i}) \quad \text{because of linearity of expectation}$$
Since the distribution y_{i} is only dependent of y_{j} and
$$\sum_{i=1}^{n} \sum_{j=1}^{m} \mathbb{E}_{y_{i}} \left[I(y_{i} = j) \middle| x_{i}, \theta^{(t)} \right] (\log w_{j} + \log \lambda_{j} - \lambda_{j} x_{i}) \quad \text{dent on } x_{i} \text{ and independent of } y_{j} \text{ and } x_{j} \text{ for } i \neq j$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{m} p\Big(y_{i} = j \middle| x_{i}, \theta^{(t)} \Big) (\log w_{j} + \log \lambda_{j} - \lambda_{j} x_{i}) \quad \text{Expectation of the indicator function of an event gives probability of that event.}$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{m} r_{ij}^{(t)} (\log w_{j} + \log \lambda_{j} - \lambda_{j} x_{i})$$

EM FOR EXPONENTIAL MIXTURE: M-STEP

Find
$$\theta^{(t+1)} = \underset{\theta}{\operatorname{arg max}} Q(\theta | \theta^{(t)})$$
 by
$$\frac{\partial}{\partial w_j} Q(\theta | \theta^{(t)}) = 0 \Rightarrow w_j = \frac{1}{n} \sum_{i=1}^n r_{ij}^{(t)}$$

$$\frac{\partial}{\partial \lambda_j} Q(\theta | \theta^{(t)}) = 0 \Rightarrow \lambda_j = \frac{\sum_{i=1}^n r_{ij}^{(t)}}{\sum_{i=1}^n r_{ij}^{(t)} \cdot x_i}$$