10-701 Introduction to Machine Learning

The EM Algorithm

Spring 2019

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(slide credit: Virginia Smith)

Outline

1. Gaussian mixture models

2. GMMs and Incomplete Data

3. EM Algorithm

EM Algorithm

EM algorithm: motivation and setup

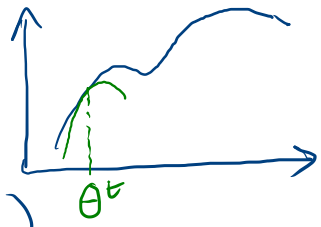
- EM is a general procedure to estimate parameters for probabilistic models with hidden/latent variables
- Suppose the model is given by a joint distribution

$$p(\boldsymbol{x}|\boldsymbol{\theta}) = \sum_{\boldsymbol{z}} p(\boldsymbol{x}, \boldsymbol{z}|\boldsymbol{\theta})$$

$p(x, z; \theta)$

$\mathcal{D} = \{x_n\}$: x : incomplete data

model: $p(x; \theta) = \sum_z p(x, z; \theta)$



$$l(\theta) = \log \prod_n p(x_n; \theta)$$

$$= \sum_n \log p(x_n; \theta)$$

$$= \sum_n \log \sum_{z_n} p(x_n, z_n; \theta)$$

$$= \sum_n \log \sum_{z_n} q_n(z_n) \frac{p(x_n, z_n; \theta)}{q_n(z_n)}$$

$$= \sum_n \log E_q\left(\frac{p(x_n, z_n; \theta)}{q_n(z_n)}\right)$$

$$\geq \sum_n E_q\left(\log\left(\frac{p(x_n, z_n; \theta)}{q_n(z_n)}\right)\right)$$

Jensen's Inequality

f: strictly concave

(i) $f(E(x)) \geq E(f(x))$

(ii) equality will hold if x is constant r.v.

$$h(\theta) = E_x\{g(x, \theta)\}$$

Equality holds if: $\frac{p(x_n, z_n; \theta^t)}{q_n(z_n)} = \text{const}$ $\forall$ values z_n

$\Rightarrow q_n(z_n) \propto p(x_n, z_n; \theta^t)$

$\Rightarrow q_n(z_n) = c\, p(x_n, z_n; \theta^t)$ $\forall$ values of z_n

$\Rightarrow \sum_{z_n} q_n(z_n) = 1 = c \sum_{z_n} p(x_n; z_n; \theta^t)$

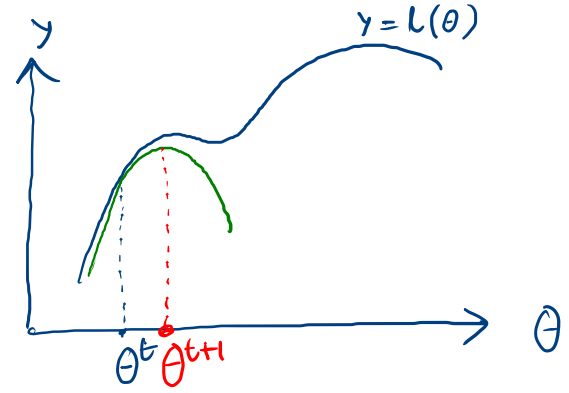
$= c\, p(x_n; \theta^t)$

$\Rightarrow c = \frac{1}{p(x_n; \theta^t)}$

$$q_n(z_n) = \frac{p(x_n, z_n; \theta^t)}{p(x_n; \theta^t)} = p(z_n | x_n; \theta^t)$$

$$l(\theta^t) = \sum_n E_q\left(\log\left(\frac{p(x_n, z_n; \theta^t)}{p(z_n | x_n; \theta^t)}\right)\right)$$

$$l(\theta) \geq \underbrace{\sum_n \sum_{z_n} p(z_n | x_n; \theta^t) \log \frac{p(x_n, z_n; \theta)}{p(z_n | x_n; \theta^t)}}_{ELBO(\theta, \theta^t)}$$



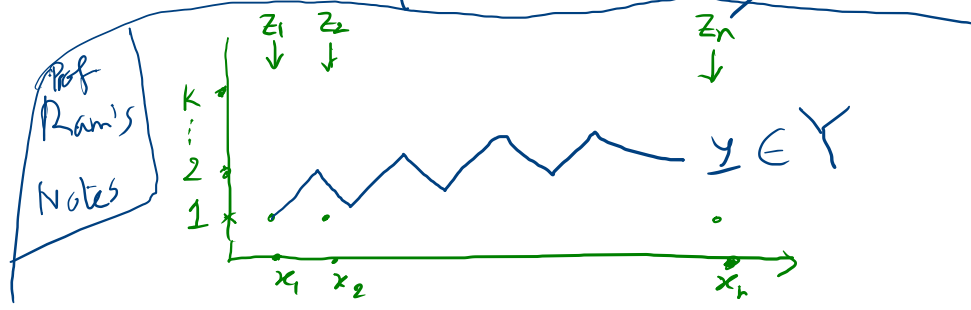
E-Step: (i) Compute the posterior $p(z_n | x_n; \theta^t)$

$$\circledast \quad Q(\theta, \theta^t) = \sum_n \sum_{z_n} p(z_n | x_n; \theta^t) \log p(x_n, z_n; \theta) = \sum_n E_q \log p(x_n, z_n; \theta)$$

$$= E_q\left(\log \prod_n (x_n, z_n; \theta)\right) \quad \leftarrow$$

M-Step:

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



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- Given **incomplete data** $\mathcal{D} = \{\boldsymbol{x}_n\}$ our goal is to compute MLE of $\boldsymbol{\theta}$:

$$\boldsymbol{\theta} = \arg\max \ell(\theta) = \arg\max \log \mathcal{D} = \arg\max \sum_n \log p(\boldsymbol{x}_n|\boldsymbol{\theta})$$

$$= \arg\max \sum_n \log \sum_{\boldsymbol{z}_n} p(\boldsymbol{x}_n, \boldsymbol{z}_n|\boldsymbol{\theta})$$

The objective function $\ell(\boldsymbol{\theta})$ is called *incomplete* log-likelihood

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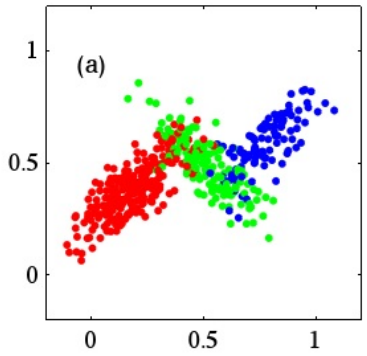
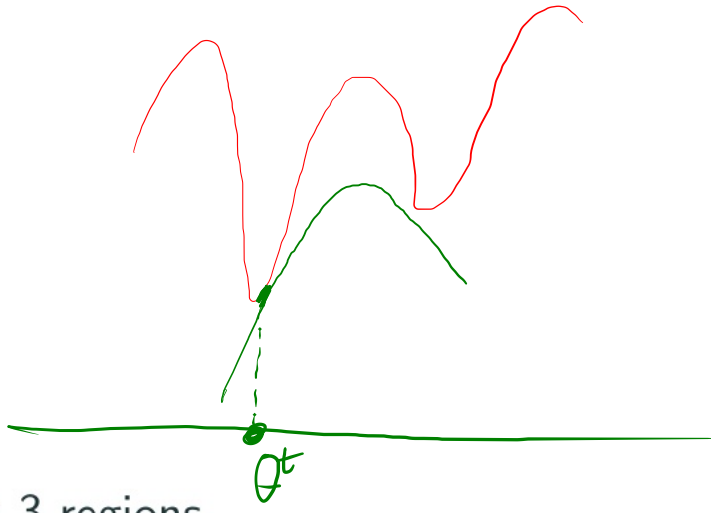
- Last step follows from Jensen's inequality, i.e., $f(\mathbb{E}X) \geq \mathbb{E}f(X)$ for concave function f

GMM Example





- Consider the previous model where $\boldsymbol{x}$ could be from 3 regions
- We can choose $q(\boldsymbol{z})$ as any valid distribution
- e.g., $q(z = k) = 1/3$ for any of 3 colors
- e.g., $q(z = k) = 1/2$ for red and blue, 0 for green

Which $q(\boldsymbol{z})$ should we choose?

Which $q(z)$ to choose?

Recall:

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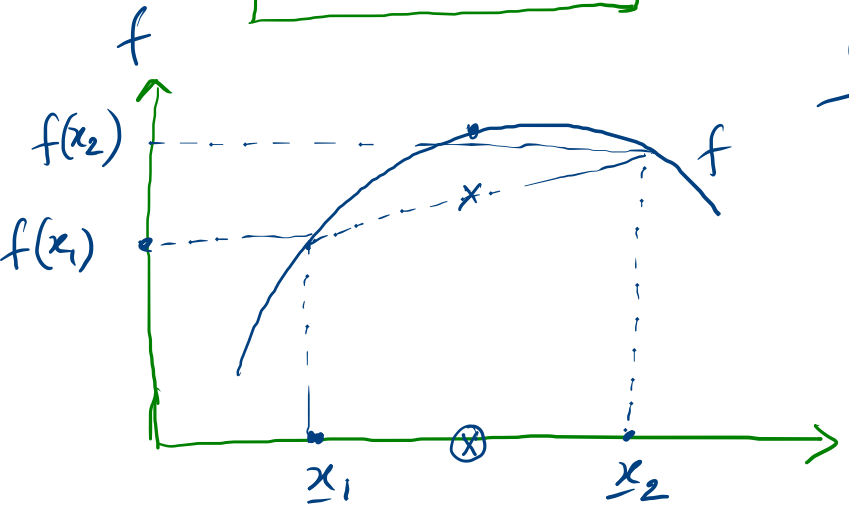

Concavity:

$$f(t\underline{x}_1 + (1-t)\underline{x}_2) \geq t\, f(\underline{x}_1) + (1-t)\, f(\underline{x}_2)$$

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- This is the **posterior distribution** of z_n given $\boldsymbol{x}_n$ and $\boldsymbol{\theta}^t$

E and M Steps

Our simplified expression

$$\ell(\boldsymbol{\theta}^t) = \sum_n \sum_{z_n} p(\boldsymbol{z}_n|\boldsymbol{x}_n;\boldsymbol{\theta}^t) \log \frac{p(\boldsymbol{x}_n, \boldsymbol{z}_n|\boldsymbol{\theta}^t)}{p(\boldsymbol{z}_n|\boldsymbol{x}_n;\boldsymbol{\theta}^t)}$$

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Why is this called the E-Step? Because we can view it as computing the *expected (complete) log-likelihood*:

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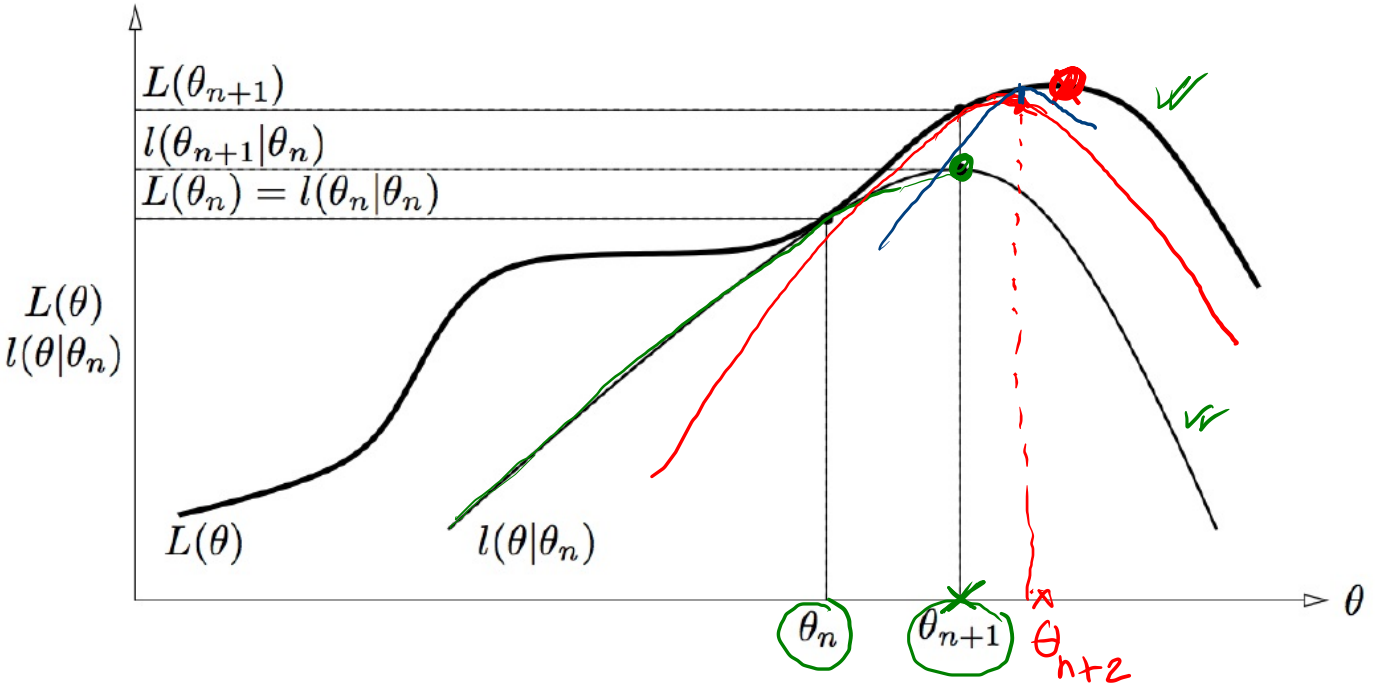
M-Step: Maximize $Q(\boldsymbol{\theta}|\boldsymbol{\theta}^t)$, i.e., $\boldsymbol{\theta}^{t+1} = \arg\max_{\boldsymbol{\theta}} Q(\boldsymbol{\theta}|\boldsymbol{\theta}^t)$

EM in Pictures



(Figure from tutorial by Sean Borman)

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- However, in the M-step, $\boldsymbol{\theta}^{t+1}$ is chosen to maximize the right hand side of the equation, thus proving our desired result

$$\ell(\theta^{t+1}) \geq \text{ELBO}(\theta, \theta^{(t+1)})$$
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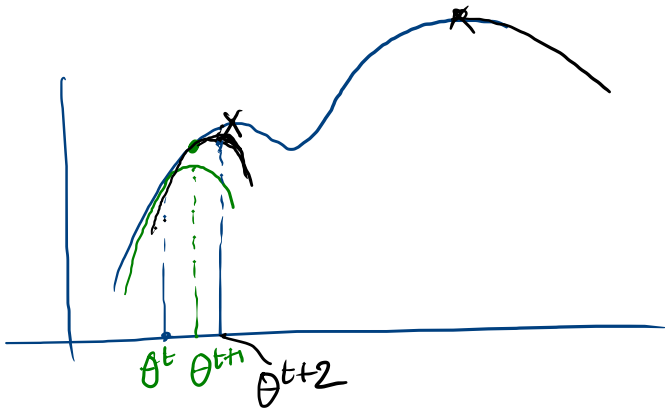

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- Note: the EM procedure converges but only to a local optimum

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  - EM is a general method to deal with hidden data; we have studied it in the context of hidden *labels* (unsupervised learning)