18-661 Introduction to Machine Learning

The EM Algorithm

Spring 2020

ECE – Carnegie Mellon University

Announcements

- HW 6 is due on Sunday, April 12.
- HW 7 will be released later this week.
  - HW 7 will be entirely focused on programming, with the goal of letting you gain experience in implementing ML models.
  - Lecture on April 13 will be a PyTorch tutorial by Ritwick. Please attend if you are not familiar with PyTorch. You will need to know your way around PyTorch for HW 7.
  - You cannot drop HW 7. Its score will be weighted equally with each of your best 5 scores from the first six homeworks to determine your overall homework grade.
- The final exam will be on Wednesday, April 29. It will have online and take-home parts.

Outline

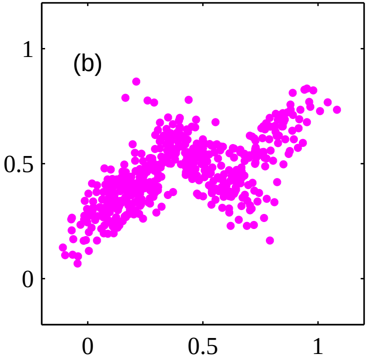
1. Recap: Gaussian Mixture Models

2. EM Algorithm

Recap: Gaussian Mixture Models

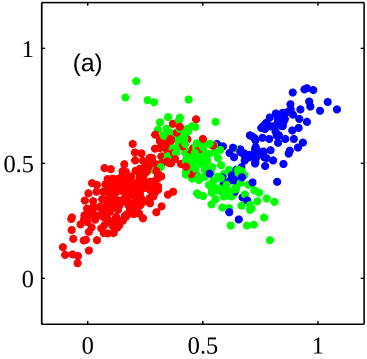
Probabilistic interpretation of clustering?

How can we model $p(\boldsymbol{x})$ to reflect our intuition that points stay close to their cluster centers?



- Points seem to form 3 clusters
- We cannot model $p(\boldsymbol{x})$ with simple and known distributions
- E.g., the data is not a Gaussian b/c we have 3 distinct concentrated regions...

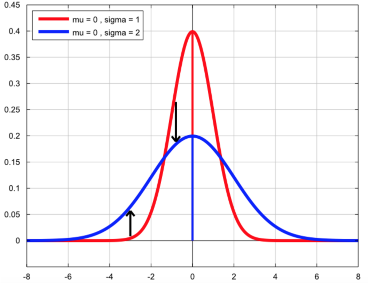
Gaussian mixture models: Intuition



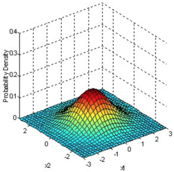
- Key idea: Model *each* region with a distinct distribution
- Can use Gaussians — Gaussian mixture models (GMMs)
- *However*, we don't know *cluster assignments* (label), *parameters* of Gaussians, or *mixture components*!
- Must learn these values from *unlabeled* data $\mathcal{D} = \{\boldsymbol{x}_n\}_{n=1}^{N}$

Recall: Gaussian (normal) distributions

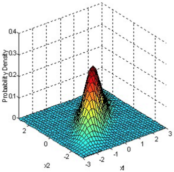
$$\mathbf{x} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \qquad f(\boldsymbol{x}) = \frac{\exp(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}))}{\sqrt{(2\pi)^n|\boldsymbol{\Sigma}|}}$$



$\boldsymbol{\mu} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \boldsymbol{\Sigma} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$



$\boldsymbol{\mu} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \boldsymbol{\Sigma} = \begin{pmatrix} 1 & 0.8 \\ 0.8 & 1 \end{pmatrix}$



Gaussian mixture models: Formal definition

GMM has the following density function for $\boldsymbol{x}$

$$p(\boldsymbol{x}) = \sum_{k=1}^{K} \omega_k N(\boldsymbol{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

- K: number of Gaussians — they are called mixture components
- $\boldsymbol{\mu}_k$ and $\boldsymbol{\Sigma}_k$: mean and covariance matrix of k-th component
- ω_k: mixture weights (or priors) represent how much each component contributes to final distribution. They satisfy 2 properties:

$$\forall\ k,\ \omega_k > 0, \quad \text{and} \quad \sum_k \omega_k = 1$$

These properties ensure $p(\boldsymbol{x})$ is in fact a probability density function.

GMM as the marginal distribution of a joint distribution

Consider the following joint distribution

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

where z is a discrete random variable taking values between 1 and K.

Denote

$$\omega_k = p(z = k)$$

Now, assume the conditional distributions are Gaussian distributions

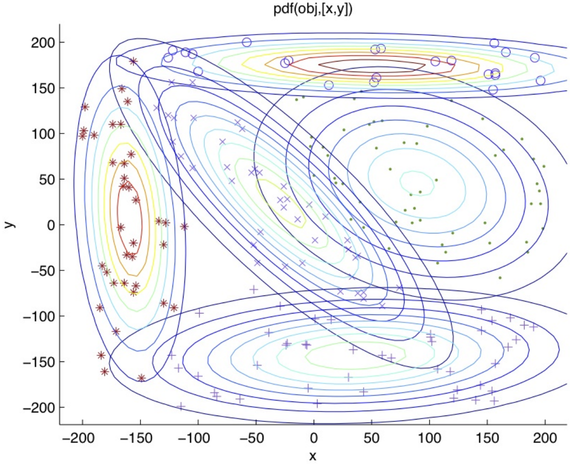
$$p(\boldsymbol{x}|z = k) = N(\boldsymbol{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

Then, the marginal distribution of $\boldsymbol{x}$ is

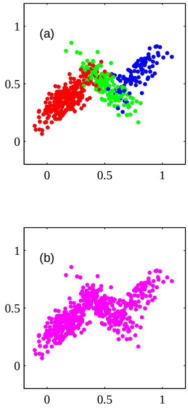
$$p(\boldsymbol{x}) = \sum_{k=1}^{K} \omega_k N(\boldsymbol{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

Namely, the Gaussian mixture model

Gaussian mixture model for clustering



GMMs: Example



The conditional distribution between $\boldsymbol{x}$ and z (representing color) are

$$\begin{aligned} p(\boldsymbol{x}|z = red) &= N(\boldsymbol{x}|\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) \\ p(\boldsymbol{x}|z = blue) &= N(\boldsymbol{x}|\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) \\ p(\boldsymbol{x}|z = green) &= N(\boldsymbol{x}|\boldsymbol{\mu}_3, \boldsymbol{\Sigma}_3) \end{aligned}$$

The marginal distribution is thus

$$\begin{aligned} p(\boldsymbol{x}) = p(z = red)&N(\boldsymbol{x}|\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) \\ + p(z = blue)&N(\boldsymbol{x}|\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) \\ + p(z = green)&N(\boldsymbol{x}|\boldsymbol{\mu}_3, \boldsymbol{\Sigma}_3) \end{aligned}$$

Parameter estimation for Gaussian mixture models

The parameters in GMMs are:

$$\boldsymbol{\theta} = \{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$$

Let's first consider the (unrealistic) case where *we know the labels z*.

Define $\mathcal{D}' = \{\boldsymbol{x}_n, z_n\}_{n=1}^N$, $\mathcal{D} = \{\boldsymbol{x}_n\}_{n=1}^N$

- $\mathcal{D}'$ is the complete data
- $\mathcal{D}$ the incomplete data

How can we learn our parameters?

Given $\mathcal{D}'$, the maximum likelihood estimation of the $\boldsymbol{\theta}$ is given by

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

Parameter estimation for GMMs: Complete data

The complete likelihood is decomposable across the labels:

$$\sum_n \log p(\boldsymbol{x}_n, z_n) = \sum_n \log p(z_n)p(\boldsymbol{x}_n|z_n) = \sum_k \sum_{n:z_n=k} \log p(z_n)p(\boldsymbol{x}_n|z_n)$$

where we have grouped data by cluster labels z_n.

Let $r_{nk} \in \{0, 1\}$ be a binary variable that indicates whether $z_n = k$:

$$\begin{aligned}\sum_n \log p(\boldsymbol{x}_n, z_n) &= \sum_k \sum_n r_{nk} \log p(z=k)p(\boldsymbol{x}_n|z=k) \\ &= \sum_k \sum_n r_{nk} \left[\log \omega_k + \log N(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\right]\end{aligned}$$

In the complete setting, the r_{nk} just add to the notation, but later we will 'relax' these variables and allow them to take on fractional values.

Parameter estimation for GMMs: Complete data

The MLE is:

$$\omega_k = \frac{\sum_n r_{nk}}{\sum_{k'} \sum_n r_{nk'}}, \quad \boldsymbol{\mu}_k = \frac{1}{\sum_n r_{nk}} \sum_n r_{nk} \boldsymbol{x}_n$$

$$\boldsymbol{\Sigma}_k = \frac{1}{\sum_n r_{nk}} \sum_n r_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top$$

Since r_{nk} is binary, the previous solution is nothing but:

- ω_k: fraction of total data points whose cluster label z_n is k
  - note that $\sum_{k'} \sum_n r_{nk'} = N$
- $\boldsymbol{\mu}_k$: mean of all data points whose label z_n is k
- $\boldsymbol{\Sigma}_k$: covariance of all data points whose label z_n is k

Parameter estimation for GMMs: Incomplete data

GMM Parameters

$$\boldsymbol{\theta} = \{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^{K}$$

Incomplete Data

Our data contains observed and unobserved data, and hence is incomplete:

- Observed: $\mathcal{D} = \{\boldsymbol{x}_n\}$
- Unobserved (hidden): $\{\boldsymbol{z}_n\}$

Goal: Obtain the maximum likelihood estimate of $\boldsymbol{\theta}$:

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

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

The objective function is called the *incomplete* log-likelihood.

Parameter estimation for GMMs: Incomplete data

No simple way to optimize the incomplete log-likelihood...

EM algorithm provides a strategy for iteratively optimizing this function!

E-Step: ‘Guess’ values of the z_n using existing values of $\boldsymbol{\theta} = \{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$. How do we do this?

When z_n is not given, we can guess it via the posterior probability (recall: Bayes’ rule!)

$$
\begin{aligned}
p(z_n = k|\boldsymbol{x}_n) &= \frac{p(\boldsymbol{x}_n|z_n = k)p(z_n = k)}{p(\boldsymbol{x}_n)} \\
&= \frac{p(\boldsymbol{x}_n|z_n = k)p(z_n = k)}{\sum_{k'=1}^K p(\boldsymbol{x}_n|z_n = k')p(z_n = k')} \\
&= \frac{N(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \times \omega_k}{\sum_{k'=1}^K N(\boldsymbol{x}_n|\boldsymbol{\mu}_{k'}, \boldsymbol{\Sigma}_{k'}) \times \omega_{k'}}
\end{aligned}
$$

Estimation with soft r_{nk}

We define $r_{nk} = p(z_n = k|\boldsymbol{x}_n)$

- Recall that r_{nk} was previously binary
- Now it's a "soft" assignment of $\boldsymbol{x}_n$ to k-th component
- Each $\boldsymbol{x}_n$ is assigned to a component fractionally according to $p(z_n = k|\boldsymbol{x}_n)$

M-Step: If we solve for the MLE of $\boldsymbol{\theta} = \{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$ given soft r_{nk}s, we get the same expressions as before!

$$\omega_k = \frac{\sum_n r_{nk}}{\sum_k \sum_n r_{nk}}, \quad \boldsymbol{\mu}_k = \frac{1}{\sum_n r_{nk}} \sum_n r_{nk} \boldsymbol{x}_n$$

$$\boldsymbol{\Sigma}_k = \frac{1}{\sum_n r_{nk}} \sum_n r_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^\top$$

But remember, we're 'cheating' by using $\boldsymbol{\theta}$ to compute r_{nk}!

EM procedure for GMM

Alternate between estimating r_{nk} and estimating parameters $\boldsymbol{\theta}$

- Step 0: Initialize $\boldsymbol{\theta}$ with some values (random or otherwise)
- Step 1: E-Step: Set $r_{nk} = p(z_n = k|\boldsymbol{x}_n)$ with the current values of $\boldsymbol{\theta}$ using Bayes Rule
- Step 2: M-Step: Update $\boldsymbol{\theta}$ using the r_{nk}s from Step 2 using MLE
- Step 3: Go back to Step 1.

At the end convert r_{nk} back to binary by setting the largest r_{nk} for point x_n to 1 and others to 0.

GMMs and K-means

GMMs provide probabilistic interpretation for K-means

GMMs reduce to K-means under the following assumptions (in which case EM for GMM parameter estimation simplifies to K-means):

- Assume all Gaussians have $\sigma^2 \boldsymbol{I}$ covariance matrices
- Further assume $\sigma \rightarrow 0$, so we only need to estimate $\boldsymbol{\mu}_k$, i.e., means

K-means is often called "hard" GMM or GMMs is called "soft" K-means

The posterior r_{nk} provides a probabilistic assignment for $\boldsymbol{x}_n$ to cluster k

GMMs vs. k-means

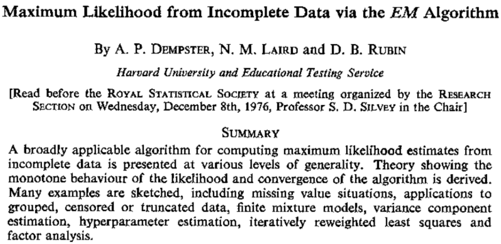
Pros/Cons

- k-means is a simpler, more straightforward method, but might not be as accurate because of deterministic clustering
- GMMs can be more accurate, as they model more information (soft clustering, variance), but can be more expensive to compute
- Both methods have a similar set of practical issues (having to select k, the distance, and the initialization)

EM Algorithm

EM algorithm: Motivation

EM is a general procedure to estimate parameters for probabilistic models with hidden/latent variables.



Maximum Likelihood from Incomplete Data via the *EM* Algorithm

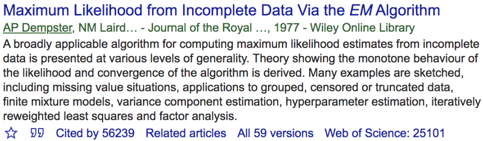
By A. P. Dempster, N. M. Laird and D. B. Rubin

Harvard University and Educational Testing Service

[Read before the Royal Statistical Society at a meeting organized by the Research Section on Wednesday, December 8th, 1976, Professor S. D. Silvey in the Chair]

Summary

A broadly applicable algorithm for computing maximum likelihood estimates from incomplete data is presented at various levels of generality. Theory showing the monotone behaviour of the likelihood and convergence of the algorithm is derived. Many examples are sketched, including missing value situations, applications to grouped, censored or truncated data, finite mixture models, variance component estimation, hyperparameter estimation, iteratively reweighted least squares and factor analysis.



Maximum Likelihood from Incomplete Data Via the *EM* Algorithm

AP Dempster, NM Laird… - Journal of the Royal …, 1977 - Wiley Online Library

A broadly applicable algorithm for computing maximum likelihood estimates from incomplete data is presented at various levels of generality. Theory showing the monotone behaviour of the likelihood and convergence of the algorithm is derived. Many examples are sketched, including missing value situations, applications to grouped, censored or truncated data, finite mixture models, variance component estimation, hyperparameter estimation, iteratively reweighted least squares and factor analysis.

☆ ” Cited by 56239 Related articles All 59 versions Web of Science: 25101

EM algorithm: Setup

- Suppose the model is given by a joint distribution

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

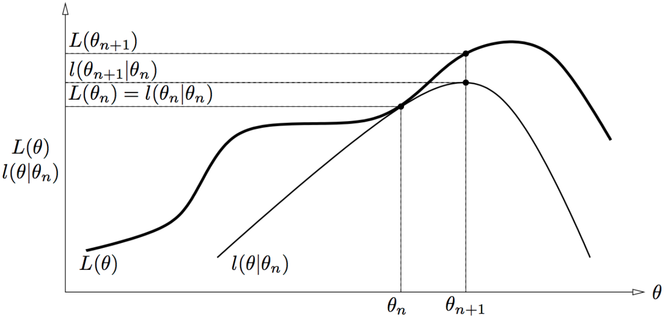
- Given incomplete data $\mathcal{D} = \{\boldsymbol{x}_n\}$ our goal is to compute MLE of $\boldsymbol{\theta}$:

$$\begin{aligned}\boldsymbol{\theta} = \arg\max \ell(\boldsymbol{\theta}) = \arg\max \log p(\mathcal{D}) &= \arg\max \sum_n \log p(\boldsymbol{x}_n|\boldsymbol{\theta}) \\ &= \arg\max \sum_n \log \sum_{\boldsymbol{z}_n} p(\boldsymbol{x}_n, \boldsymbol{z}_n|\boldsymbol{\theta})\end{aligned}$$

- The objective function $\ell(\boldsymbol{\theta})$ is called *incomplete* log-likelihood
- log-sum form of incomplete log-likelihood is difficult to work with

EM: Principle

- EM: construct lower bound on $\ell(\boldsymbol{\theta})$ (E-step) and optimize it (M-step)
- "Majorization-minimization (MM)"
- Optimizing the lower bound will hopefully optimize $\ell(\boldsymbol{\theta})$ too.



(Figure from tutorial by Sean Borman)

Constructing a lower bound

- If we define $q(\boldsymbol{z})$ as a distribution over $\boldsymbol{z}$, then

$$\begin{aligned}\ell(\boldsymbol{\theta}) &= \sum_n \log \sum_{\boldsymbol{z}_n} p(\boldsymbol{x}_n, \boldsymbol{z}_n | \boldsymbol{\theta}) \\ &= \sum_n \log \sum_{\boldsymbol{z}_n} q(\boldsymbol{z}_n) \frac{p(\boldsymbol{x}_n, \boldsymbol{z}_n | \boldsymbol{\theta})}{q(\boldsymbol{z}_n)} \\ &\geq \sum_n \sum_{\boldsymbol{z}_n} q(\boldsymbol{z}_n) \log \frac{p(\boldsymbol{x}_n, \boldsymbol{z}_n | \boldsymbol{\theta})}{q(\boldsymbol{z}_n)}\end{aligned}$$

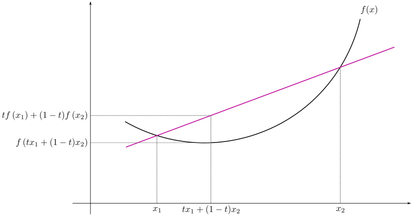
- Last step follows from Jensen's inequality, i.e., $f(\mathbb{E}X) \geq \mathbb{E}f(X)$ for concave function $f(x) = \log(x)$.

Detour: Jensen's inequality

Jensen's inequality: if $f(\cdot)$ is a *convex* function, then for any random variable X

$$f(\mathbb{E}X) \leq \mathbb{E}f(X)$$

where equality holds when $f(\cdot)$ is a constant function.



- Example: for $f(x) = x^2$ which is convex:

$$(\mathbb{E}X)^2 \leq \mathbb{E}X^2 \Longrightarrow \mathrm{Var}(X) = \mathbb{E}X^2 - (\mathbb{E}X)^2 \geq 0$$

- Example: for $f(x) = \log x$ which is *concave*:

$$\log(\mathbb{E}X) \geq \mathbb{E}\log(X)$$

Applying Jensen's inequality

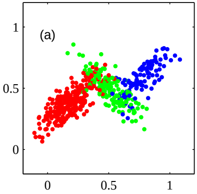
If we define $q(\boldsymbol{z})$ as a distribution over $\boldsymbol{z}$, then

$$\begin{aligned}\ell(\boldsymbol{\theta}) &= \sum_n \log \sum_{\boldsymbol{z}_n} p(\boldsymbol{x}_n, \boldsymbol{z}_n|\boldsymbol{\theta}) \\ &= \sum_n \underbrace{\log \sum_{\boldsymbol{z}_n} q(\boldsymbol{z}_n) \frac{p(\boldsymbol{x}_n, \boldsymbol{z}_n|\boldsymbol{\theta})}{q(\boldsymbol{z}_n)}}_{f\left(\mathbb{E}_{q(\boldsymbol{z}_n)}\left[\frac{p(\boldsymbol{x}_n, \boldsymbol{z}_n|\boldsymbol{\theta})}{q(\boldsymbol{z}_n)}\right]\right)}\end{aligned}$$

Apply Jensen's inequality to each term, i.e., $f(\mathbb{E}X) \geq \mathbb{E}f(X)$, for concave function $f(\cdot) = \log(\cdot)$. We take the expectation of $X = \frac{p(\boldsymbol{x}_n, \boldsymbol{z}_n|\boldsymbol{\theta})}{q(\boldsymbol{z}_n)}$, a random variable depending on $\boldsymbol{z}_n$, over the probability distribution $q(\boldsymbol{z}_n)$.

$$\ell(\boldsymbol{\theta}) \geq \sum_n \underbrace{\sum_{\boldsymbol{z}_n} q(\boldsymbol{z}_n) \log \frac{p(\boldsymbol{x}_n, \boldsymbol{z}_n|\boldsymbol{\theta})}{q(\boldsymbol{z}_n)}}_{\mathbb{E}_{q(\boldsymbol{z}_n)}\left[f\left(\frac{p(\boldsymbol{x}_n, \boldsymbol{z}_n|\boldsymbol{\theta})}{q(\boldsymbol{z}_n)}\right)\right]}$$

Which $q(z)$ should we choose?



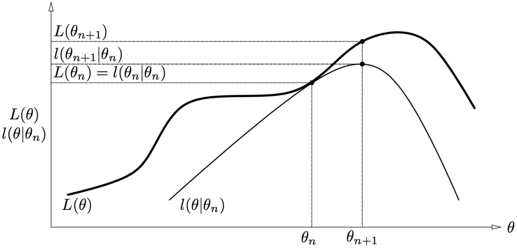
- Consider the previous model where $\boldsymbol{x}$ could be from 3 regions
- We can choose $q(\boldsymbol{z})$ as any valid distribution
- e.g., $q(z = k) = 1/3$ for any of 3 colors
- e.g., $q(z = k) = 1/2$ for red and blue, 0 for green

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

Which $q(z)$ to choose?

$$\ell(\boldsymbol{\theta}) \geq \sum_n \sum_{\boldsymbol{z}_n} q(\boldsymbol{z}_n) \log \frac{p(\boldsymbol{x}_n, \boldsymbol{z}_n | \boldsymbol{\theta})}{q(\boldsymbol{z}_n)}$$

- The lower bound we derived for $\ell(\boldsymbol{\theta})$ holds for all choices of $q(\cdot)$
- We want a tight lower bound, so given some current estimate $\boldsymbol{\theta}^t$, we will pick $q_t(\cdot)$ such that our lower bound holds with equality at $\boldsymbol{\theta}^t$.
- We will choose a *different* $q_t(\cdot)$ *for each iteration* t.



(Figure from tutorial by Sean Borman)

Pick $q_t(z_n)$

Pick $q_t(\boldsymbol{z}_n)$ so that

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

- Pick the distribution where the equality in Jensen's inequality holds.
- Choose $q_t(\boldsymbol{z}_n) \propto p(\boldsymbol{x}_n, \boldsymbol{z}_n | \boldsymbol{\theta}^t)$!
- Since $q_t(\cdot)$ is a distribution, we have

$$q_t(\boldsymbol{z}_n) = \frac{p(\boldsymbol{x}_n, \boldsymbol{z}_n | \boldsymbol{\theta}^t)}{\sum_k p(\boldsymbol{x}_n, z_n = k | \boldsymbol{\theta}^t)} = \frac{p(\boldsymbol{x}_n, \boldsymbol{z}_n | \boldsymbol{\theta}^t)}{p(\boldsymbol{x}_n | \boldsymbol{\theta}^t)} = p(\boldsymbol{z}_n | \boldsymbol{x}_n; \boldsymbol{\theta}^t)$$

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

E-Step in GMMs

GMM Parameters

$$\boldsymbol{\theta} = \{\omega_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^{K}$$

Incomplete Data

Our data contains observed and unobserved data, and hence is incomplete

- Observed: $\mathcal{D} = \{\boldsymbol{x}_n\}$
- Unobserved (hidden) labels: $\{\boldsymbol{z}_n\}$

Guess the distribution of $\boldsymbol{z}_n$ with the posterior probabilities, given estimates of $\boldsymbol{\theta}^t$:

$$\begin{aligned} q_t(\boldsymbol{z}_n) = p(\boldsymbol{z}_n = k|\boldsymbol{x}_n; \boldsymbol{\theta}^t) &= \frac{p(\boldsymbol{x}_n|z_n = k)p(z_n = k)}{\sum_{k'=1}^{K} p(\boldsymbol{x}_n|z_n = k')p(z_n = k')} \\ &= \frac{N(\boldsymbol{x}_n|\boldsymbol{\mu}_k^t, \boldsymbol{\Sigma}_k^t) \times \omega_k^t}{\sum_{k'=1}^{K} N(\boldsymbol{x}_n|\boldsymbol{\mu}_{k'}^t, \boldsymbol{\Sigma}_{k'}^t) \times \omega_{k'}^t} \end{aligned}$$

E- and M-Steps

Our lower bound for the log-likelihood:

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

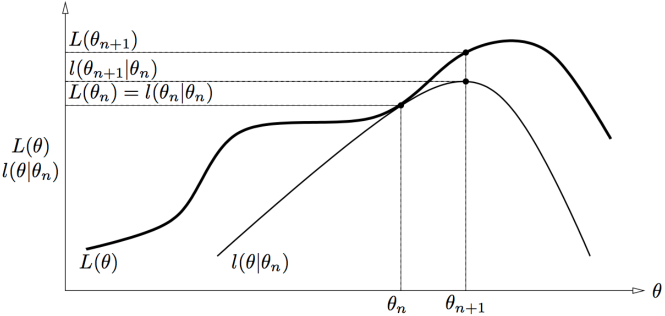
Why is this called the E-Step? Because we can view it as computing the *expected (complete) log-likelihood*:

$$Q(\boldsymbol{\theta}|\boldsymbol{\theta}^t) = \sum_n \sum_{\boldsymbol{z}_n} p(\boldsymbol{z}_n|\boldsymbol{x}_n; \boldsymbol{\theta}^t) \underbrace{\log p(\boldsymbol{x}_n, \boldsymbol{z}_n|\boldsymbol{\theta})}_{\text{complete log-likelihood}} = \mathbb{E}_{q_t} \sum_n \log p(\boldsymbol{x}_n, \boldsymbol{z}_n|\boldsymbol{\theta})$$

Where did the $p(\boldsymbol{z}_n|\boldsymbol{x}_n; \boldsymbol{\theta}^t)$ in the denominator go? It is not a function of $\boldsymbol{\theta}$, so can be ignored.

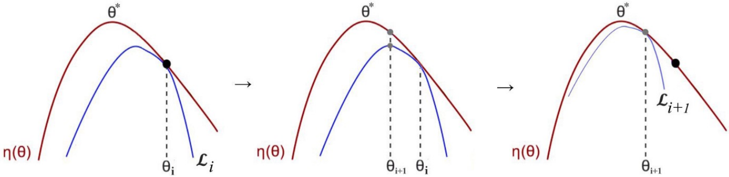
M-Step: Maximize $Q(\boldsymbol{\theta}|\boldsymbol{\theta}^t)$, i.e., $\boldsymbol{\theta}^{t+1} = \arg\max_{\boldsymbol{\theta}} Q(\boldsymbol{\theta}|\boldsymbol{\theta}^t)$

EM in Pictures



(Figure from tutorial by Sean Borman)

EM in Pictures



Adapted from Jonathan Hui's Medium tutorial.

Iterative and monotonic improvement

$$\ell(\boldsymbol{\theta}) \geq \underbrace{\sum_n \sum_{\boldsymbol{z}_n} p(\boldsymbol{z}_n|\boldsymbol{x}_n;\boldsymbol{\theta}^t) \log \frac{p(\boldsymbol{x}_n, \boldsymbol{z}_n|\boldsymbol{\theta})}{p(\boldsymbol{z}_n|\boldsymbol{x}_n;\boldsymbol{\theta}^t)}}_{Q(\boldsymbol{\theta}|\boldsymbol{\theta}^t)}$$

- We can show that $\ell(\boldsymbol{\theta}^{t+1}) \geq \ell(\boldsymbol{\theta}^t)$.
- Recall that we chose $q_t(\cdot)$ in the E-Step such that:

$$\ell(\boldsymbol{\theta}^t) = Q(\boldsymbol{\theta}^t|\boldsymbol{\theta}^t)$$

- However, in the M-step, $\boldsymbol{\theta}^{t+1}$ is chosen to maximize $Q(\boldsymbol{\theta}|\boldsymbol{\theta}^t)$, thus

$$\ell(\boldsymbol{\theta}^{t+1}) \geq Q(\boldsymbol{\theta}^{t+1}|\boldsymbol{\theta}^t) = \max_{\boldsymbol{\theta}} Q(\boldsymbol{\theta}|\boldsymbol{\theta}^t) \geq Q(\boldsymbol{\theta}^t|\boldsymbol{\theta}^t) = \ell(\boldsymbol{\theta}^t)$$

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

Example: Applying EM to GMMs

What is the E-Step in GMM?

$$r_{nk} = p(z = k | \boldsymbol{x}_n; \boldsymbol{\theta}^t)$$

What is the M-Step in GMM? The Q-function is

$$\begin{aligned}
Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)}) &= \sum_n \sum_k p(z = k|\boldsymbol{x}_n; \boldsymbol{\theta}^t) \log p(\boldsymbol{x}_n, z = k|\boldsymbol{\theta}) \\
&= \sum_n \sum_k r_{nk} \log p(\boldsymbol{x}_n, z = k|\boldsymbol{\theta}) \\
&= \sum_k \sum_n r_{nk} \log p(z = k) p(\boldsymbol{x}_n|z = k) \\
&= \sum_k \sum_n r_{nk} \left[\log \omega_k + \log N(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\right]
\end{aligned}$$

We have recovered the parameter estimation algorithm for GMMs that we previously discussed!

Example: Estimating height distributions

Suppose the heights of men and women follow two normal distributions with different parameters:

$$\text{Men} : N(\mu_1, \sigma_1^2) \quad \text{Women} : N(\mu_2, \sigma_2^2)$$

Our data, x_n, $n = 1, 2, \ldots, 5$ is the heights of five people: 179, 165, 175, 185, 158 (in cm).

We are missing the labels $z_n =$ each person's gender. Let π equal the fraction of males in the population.

How do we estimate $\mu_1, \sigma_1, \mu_2, \sigma_2, \pi$?

Example taken from: `http://web1.sph.emory.edu/users/hwu30/teaching/statcomp/Notes/Lecture3_EM.pdf`

Example: E-Step

Initialize $\mu_1^0 = 175$, $\mu_2^0 = 165$, $\sigma_1^0 = \sigma_2^0 = 10$, $\pi^0 = 0.6$.

E-Step: Estimate the probability of each person being male or female.

$$p(z_n = \mathrm{male}|\mu_1, \sigma_1, \mu_2, \sigma_2, \pi) = \frac{0.6 \exp\left[\frac{-(x_n - 175)^2}{200}\right]}{0.6 \exp\left[\frac{-(x_n - 175)^2}{200}\right] + 0.4 \exp\left[\frac{-(x_n - 165)^2}{200}\right]}$$

$$p(z_n = \mathrm{female}|\mu_1, \sigma_1, \mu_2, \sigma_2, \pi) = 1 - p(z_n = \mathrm{male}|\mu_1, \sigma_1, \mu_2, \sigma_2, \pi)$$

Person	1	2	3	4	5
x_i: height	179	165	175	185	158
Prob. male	0.79	0.48	0.71	0.87	0.31

We can use these probabilities to find $Q(\boldsymbol{\theta}^1|\boldsymbol{\theta}^0)$.

Example: M-Step

M-Step: Find $\mu_1^1, \mu_2^1, \sigma_1^1, \sigma_2^1, \pi^1$ that maximize $Q(\boldsymbol{\theta}^1|\boldsymbol{\theta}^0)$:

$$\mu_1^1 = \frac{\sum_{n=1}^5 p(z_n = \text{male}|\boldsymbol{\theta}^0) x_n}{\sum_{n=1}^5 p(z_n = \text{male}|\boldsymbol{\theta}^0)}, \; \mu_2^1 = \frac{\sum_{n=1}^5 p(z_n = \text{female}|\boldsymbol{\theta}^0) x_n}{\sum_{n=1}^5 p(z_n = \text{female}|\boldsymbol{\theta}^0)},$$

$$\sigma_1^1 = \frac{\sum_{n=1}^5 p(z_n = \text{male}|\boldsymbol{\theta}^0)(x_n - \mu_1^1)^2}{\sum_{n=1}^5 p(z_n = \text{male}|\boldsymbol{\theta}^0)},$$

$$\sigma_2^1 = \frac{\sum_{n=1}^5 p(z_n = \text{female}|\boldsymbol{\theta}^0)(x_n - \mu_2^1)^2}{\sum_{n=1}^5 p(z_n = \text{female}|\boldsymbol{\theta}^0)},$$

$$\pi^1 = \frac{1}{5} \sum_{n=1}^5 p(z_n = \text{male}|\boldsymbol{\theta}^0)$$

Here we are using the MLE solution that we derived earlier for GMMs.

Numerically, $\mu_1^1 = 176$, $\mu_2^1 = 167$, $\sigma_1^1 = 8.7$, $\sigma_2^1 = 9.2$, $\pi^1 = 0.63$.

Example: After 15 iterations...

After iteration 1:

Person	1	2	3	4	5
x_1: height	179	165	175	185	158
Prob. male	0.79	0.48	0.71	0.87	0.31

Parameter estimates: $\mu_1^1 = 176$, $\mu_2^1 = 167$, $\sigma_1^1 = 8.7$, $\sigma_2^1 = 9.2$, $\pi^1 = 0.63$.

After iteration 15:

Person	1	2	3	4	5
x_1: height	179	165	175	185	158
Prob. male	0.999997	0.0004009	0.9991	1	2.44e-06

Final estimates: $\mu_1 = 179.6$, $\mu_2 = 161.5$, $\sigma_1 = 4.1$, $\sigma_2 = 3.5$, $\pi = 0.6$.

Another example: Multinomial distributions

Suppose we are trying to model the number of people who will vote for one of four candidates. We know that the probability of a single person voting for each candidate is:

$$(p_1, p_2, p_3, p_4) = \left(\frac{1}{2} + \frac{\theta}{4}, \frac{1-\theta}{4}, \frac{1-\theta}{4}, \frac{\theta}{4}\right).$$

Let $Y = (y_1, y_2, y_3, y_4)$ denote our observation of the number of votes for each candidate. How do we estimate θ?

- Option 1: MLE. But it is hard to optimize the log-likelihood...

$$\log p(Y|\theta) = y_1 \log\left(\frac{1}{2} + \frac{\theta}{4}\right) + (y_2 + y_3)\log(1-\theta) + y_4 \log\theta$$

- Option 2: EM. We will introduce two *unobserved/latent variables* x_0 and x_1, where $x_0 + x_1 = y_1$. In other words, y_1 combines the counts of two categories, whose individual counts are given by x_0 and x_1. We have a probability $\frac{1}{2}$ of picking the x_0 category, and a probability $\frac{\theta}{4}$ of picking the x_1 category.

Applying EM to multinomial distributions

Complete likelihood function:

$$\ell(\theta) = \log p(X, Y|\theta) = (x_1 + y_4)\log\theta + (y_2 + y_3)\log(1-\theta)$$

E-Step: Find $Q(\theta|\theta^t) = \mathbb{E}_{q_t}[\ell(\theta)]$, where q_t is the posterior distribution of x_1 given $y_1, y_2, y_3, y_4, \theta$. To do this, we need to find $\mathbb{E}_{q_t}[x_1]$:

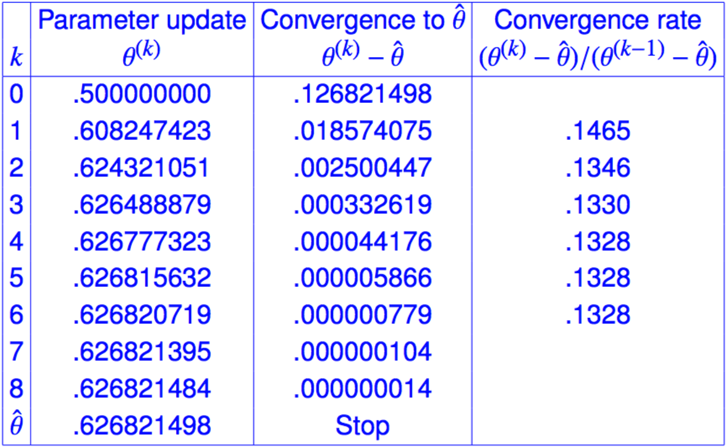
$$x_1^{t+1} = \mathbb{E}_{q_t}[x_1] = y_1 \frac{\frac{\theta^t}{4}}{\frac{1}{2} + \frac{\theta^t}{4}}.$$

M-Step: Find θ that maximizes
$Q(\theta|\theta^t) = \left(y_1 \frac{\frac{\theta^t}{4}}{\frac{1}{2}+\frac{\theta^t}{4}} + y_4\right)\log\theta + (y_2 + y_3)\log(1-\theta).$

$$\theta^{t+1} = \frac{x_1^{t+1} + y_4}{x_1^{t+1} + y_4 + y_2 + y_3}$$

What does this look like in practice?

Observe $Y = (125, 18, 20, 34)$ and initialize $\theta^0 = 0.5$.



	Parameter update	Convergence to $\hat{\theta}$	Convergence rate
k	$\theta^{(k)}$	$\theta^{(k)} - \hat{\theta}$	$(\theta^{(k)} - \hat{\theta})/(\theta^{(k-1)} - \hat{\theta})$
0	.500000000	.126821498	
1	.608247423	.018574075	.1465
2	.624321051	.002500447	.1346
3	.626488879	.000332619	.1330
4	.626777323	.000044176	.1328
5	.626815632	.000005866	.1328
6	.626820719	.000000779	.1328
7	.626821395	.000000104	
8	.626821484	.000000014	
$\hat{\theta}$	.626821498	Stop	

Applications of EM

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

- Filling in missing data in a sample
- Discovering the value of latent model variables
- Estimating parameters of finite mixture models
- As an alternative to direct maximum likelihood estimation

You should know . . .

- EM is a general procedure for maximizing a likelihood with *latent (unobserved) variables*
- The two steps of EM:
  - (1) Estimating unobserved data from observed data and current parameters
  - (2) Using this “complete” data to find the maximum likelihood parameter estimates
- Pros: Guaranteed to converge, no parameters to tune (e.g., compared to gradient methods)
- Cons: Can get stuck in local optima, can be expensive