Lecture 15 - EM Algorithm

Keck School of
Medicine of USC

Final exam

- When: **Friday May 6th** at 10am.
- What: 5-7 minute presentation each. (Can join with 1 or 2 others if you prefer.)
- Where: Zoom (room details will be on Blackboard under ZoomPro tab).
- I will be strict with timing so that we are not there all day (with apologies).
- Each person will share their screen when presenting
- Please have fun with it!

The Expectation-Maximization (EM) algorithm

The expectation maximization algorithm is a natural generalization of maximum likelihood estimation to the incomplete data case. – Chuong B Do & Serafim Batzoglou. What is the expectation maximization algorithm? Nature Biotechnology. 2008.

Overall

- A general framework, introduced by Laird and Rubin (1977) to encompass a variety of problems:
  - Filling in missing data
  - Inferring latent variables
  - Estimating HMM parameters
  - Estimating parameters for mixture models
  - Unsupervised cluster learning

EM had been around for a while before it was formally 'christened'…

Newcomb (1887)
McKendrick (1926)
Hartley (1958)
Baum et al. (1970) [The HMM Baum-Welch algorithm is an EM algorithm!]

Canonical example

- Have a mixture distribution.
- Don't know which points belong to which components of the mixture.
- Wish to estimate parameters of underlying mixture (or assign points probabilistically to the mixture components).

Motivating example

- Imagine we have two coins, for each of which the prob. of getting a "Heads", p_1 , p_2, is unknown.
- Suppose we repeat the following n times:
  - Pick a coin, uniformly at random, and toss it m times, recording the outcome.
- We can construct the maximum likelihood estimators of p_1 & p_2 as
  - MLE of p_1 = proportion of tosses of coin 1 that resulted in a "Heads".
- *But what if we don't know which coin was chosen for each of the n trials?*

Motivating example

- Possible approach:
  1. Choose initial values for p_1 & p_2.
  2. Given those values, find the prob. that each of the n trials used coin 1. (Bayes' theorem). Call these numbers $\pi_1,\ldots,\pi_n$
  3. For each i, if $\pi_i > 0.5$ assign the i^{th} trial to coin 1; otherwise assign it to coin 2.
  4. Re-estimate p_1 & p_2 assuming the assignments in step 3 were correct.
  5. Repeat steps 2-4 until the estimates for p_1 & p_2 converge.

[This is essentially a version of k-means clustering.]

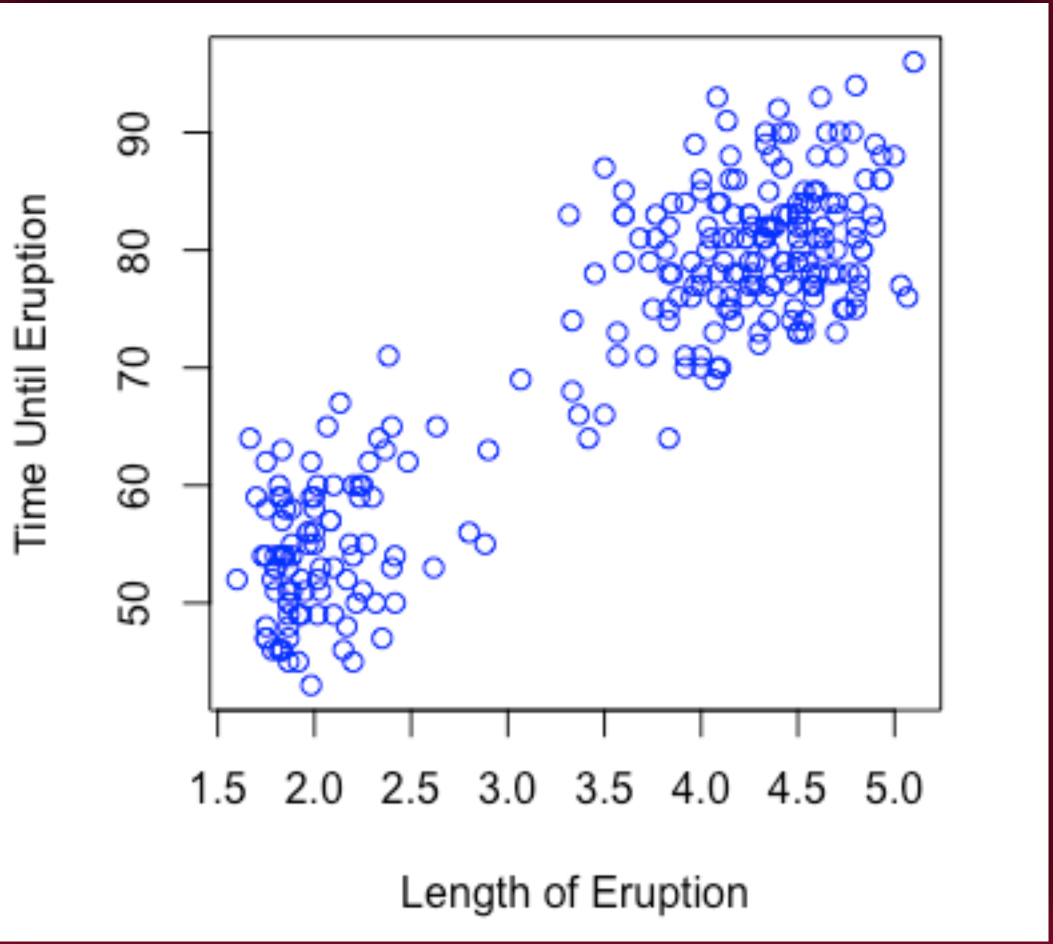
Motivating example

- The EM algorithm does the same thing, but with "soft" assignments.
- So for each trial, i, we would say it has probability π_I of being generated by coin 1 and $(1-\pi_i)$ of being generated by coin 2.
- We then repeat the algorithm on the previous page, but maximizing the likelihood for p_1 and p_2 using these *soft* assignments. So we get terms like

$$P(HTTHH \mid \text{trial } i) = \pi_i p_1^3(1-p_1)^2+(1-\pi_i)p_2^3(1-p_2)^2$$

in the likelihood term that we are maximizing with respect to p_1 and p_2.

Old Faithful



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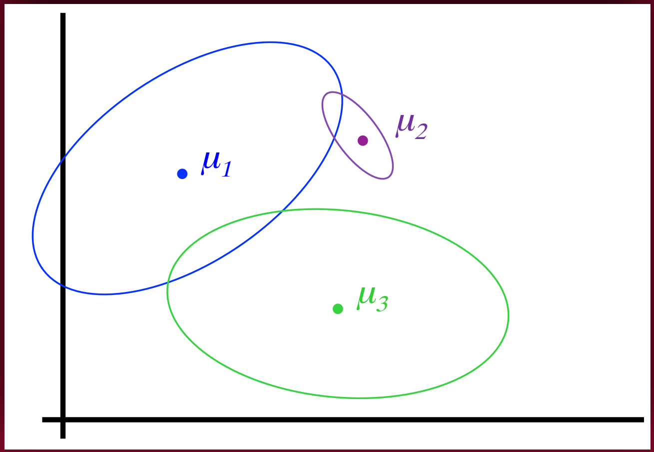
Gaussian Mixture Model example



Underlying assumptions:

1. There are k components
2. Each point is generated by:
   - Sampling a component Y with prob. P(Y)
   - Sampling from $N(\mu_i, \sigma_i^2)$

Probability model

- So, in general, for each datapoint, x, we will have:

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \underbrace{\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}_{\text{Component}}$$

Mixing coefficient

$$\forall k : \pi_k \geqslant 0 \qquad \sum_{k=1}^{K} \pi_k = 1$$

Maximum likelihood

- The EM algorithm, seeks to maximize the marginal likelihood:

$$\text{argmax}_\theta \prod_j P(x_j) = \text{argmax}_\theta \prod_j \sum_{k=1}^{K} P(Y_j=k, x_j)$$

where Y_j is the cluster to which x_j is probabilistically assigned.

E-M algorithm

- The algorithm alternates between two steps:
  - Expectation - compute conditional probs. to **probabilistically** fill in missing (unobserved) values conditional on the current parameters.
  - Maximization - re-estimate the parameters conditional on the current **probabilistic** assignments (using maximum likelihood).

EM algorithm - mixture models

- E step: Calculate $P(Y_j=k \mid x_j,\theta)$.
- M step:

  Set $\theta = \mathrm{argmax}_\theta \sum_j \sum_k P(Y_j=k \mid x_{j,} \theta) \log P(Y_j=k, x_j \mid \theta)$

X_j = the datapoints
Y_j = cluster to which x_j is assigned (probabilistic!)
θ = parameters (Normal means and variances here)
K = cluster index

EM algorithm - mixture models

- E-step:
  - Compute 'expected' clusters of all datapoints

$$P\left(Y_j = k \middle| x_j, \mu_1 \ldots \mu_K\right) \propto \exp\left(-\frac{1}{2\sigma^2}\left\|x_j - \mu_k\right\|^2\right)\mathrm{P}\left(Y_j = k\right)$$

EM algorithm - mixture models

- M-step:
  - Compute most likely cluster means given current assignments:

$$\mu_k = \frac{\sum_{j=1}^{m} P\left(Y_j = k \middle| x_j\right) x_j}{\sum_{j=1}^{m} P\left(Y_j = k \middle| x_j\right)}$$

EM Algorithm

- See examples in EM_Algorithm repo from week 15.
- **Note:** convergence is only guaranteed to a local maximum, so run the algorithm multiple times from different start points.
- Further reading: “What is the expectation maximization algorithm?” Chuong B Do & Serafim Batzoglou, Nature Biotechnology, volume 26, pages 897–899 (2008)

END