The EM algorithm I: introduction

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Overview

Today, we cover:

- The EM Algorithm: intro and applications
- Review of some MLE theory

Announcements

- HW3 posted and due 3/4 at 10:00AM

Readings:

- Chapter 4: The EM Algorithm, in Peng
- Givens and Hoeting Chapter 4

Last lectures

- General optimization problems
  - Steepest descent
  - Newton's method
  - Fisher scoring
  - Quasi-Newton
- GLMs
  - iteratively reweighted least squares

Expectation–maximization (EM) algorithm

- An iterative algorithm for **maximizing likelihood** when the model contains unobserved latent variables
- The algorithm iterates between **E-step** (expectation) and **M-step** (maximization)
- **E-step**: fill in the missing/latent values
- **M-step**: obtain parameters maximizing the expected log-likelihood from the E step

EM algorithm

Widely used algorithm!! Some common uses include:

- Gaussian mixture models
- Hidden Markov models
- Missing data imputation
- Latent variable models (i.e. factor analysis, latent growth curves)
- Censored or truncated data

EM algorithm

Pros

- Guarantees monotone improvement of the likelihood function
- Handles missing data

Cons

- Convergence is to a local, not necessarily global, solution
    - Can be heavily dependent on initial values
- Convergence can be slow, especially for high-dimensional problems (lots of parameters)

EM: notation

- Y: observed data vector
- Z: vector of data that are missing
- θ: vector of parameters we want to estimate
- $p(y, z|\theta)$: complete data density
- $p(y|\theta) = \int_z p(y, z|\theta) dz$: observed data density
    - $l(\theta|y) = \log f(y|\theta)$: observed data likelihood
- $p(z|y, \theta)$: conditional density of missing data given observed data

EM: intuition

Idea: In order to estimate θ via MLE *using only the observed data*, need to be able to maximize $l(\theta|y) = \log f(y|\theta) = \int_z p(y, z|\theta)dz$

- BUT $l(\theta|y)$ difficult to maximize because of the integral
- INSTEAD: assuming $p(y, z|\theta)$ has some nice form (like EF)
  - If we have estimate of missing data Z, can easily evaluate $p(y, z|\theta)$

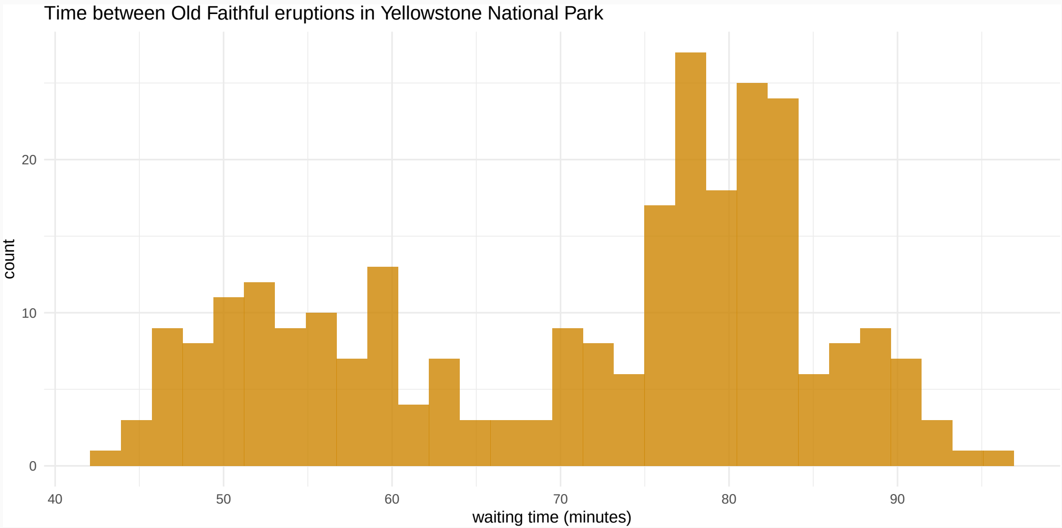
To do this, we construct surrogate function (called Q function)

- Q is expected value of log likelihood for $p(y, z|\theta)$ *with respect to conditional distribution of missing given observed data*, $p(z|y, \theta)$, for current estimate of parameters, θ_0
- **M-Step** maximizes this surrogate function
  - Akin to filling in the missing data then taking the MLE for θ

Canonical examples

- Two-part Gaussian mixture model
  - Data $Y_1, \ldots, Y_n$ come from a mixture of two Gaussian distributions
  - Soft clustering/unsupervised learning technique
  - **Example**: A new blood biomarker shows promise as an early Alzeimer's detection biomarker. Values of the biomarker in a sample of patients have a bimodal distribution: healthy subjects, those with Alzeimers
  - **Example**: a clinical trial is evaluating response to a new cancer drug. There are three subpopulations: non-responders, partial responders, complete responders
- Censored exponential data

Example: Old Faithful waiting times



EM: steps

(1) **E-Step**: Let θ_0 be the current estimate of θ. Define

$$Q(\theta|\theta_0) = E_z\left[\log p(y, z|\theta)|y, \theta_0\right]$$

(2) **M-Step**: Maximize $Q(\theta|\theta_0)$ with respect to θ to get next value of θ

(3) Iterate between E and M steps until convergence.

Note: E-step expectation taken WRT missing data density,

$$p(z|y, \theta) = \frac{p(y, z|\theta)}{p(y|\theta)}$$

EM: convergence

How to monitor convergence in EM?

- Each iteration is designed to increase the **observed data log likelihood**, $p(y|\theta)$.
    - Check if falls below a certain threshold, then stop
        - $p(y|\theta^{k+1}) - p(y|\theta^{k}) < \epsilon$
- In practice, can be very sensitive to starting values
    - Can fail due to numerical difficulties if starting values are far from the truth

However, $p(y|\theta)$ **cannot always be computed**!

- Another option: $(\theta^{t+1} - \theta^{t})^{T}(\theta^{t+1} - \theta^{t}) < \epsilon$
- Another option: $|Q(\theta^{t+1}|\theta^{t}) - Q(\theta^{t}|\theta^{t})| < \epsilon$

Two-part Gaussian mixture model

- $Y_1, \dots, Y_n$ are sampled independently from a mixture of two Normal distributions with density

$$p(y|\theta) = \lambda \mathcal{N}(y|\mu_1, \sigma_1^2) + (1-\lambda)\mathcal{N}(y|\mu_2, \sigma_2^2)$$

- $\theta = (\mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \lambda)$
- $Z_1, \dots, Z_n$: labels identifying which observation came from which population
    - $Z_i = 1$ if Y_i from $\mathcal{N}(y|\mu_1, \sigma_1^2)$; $Z_i = 0$ otherwise

$$z_i \sim Bernoulli(\lambda)$$

Two-part Gaussian mixture model

Joint density of observed and missing data (i.e. complete data density) is then

$$p(y, z|\theta) = \left[\lambda \mathcal{N}(y|\mu_1, \sigma_1^2)\right]^z \left[(1-\lambda)\mathcal{N}(y|\mu_2, \sigma_2^2)\right]^{1-z}$$

Exercise: show that integrating out the missing data gives the observed data density

Two-part Gaussian mixture model

Two-part Gaussian mixture model

Then, complete-data log likelihood is

$$\log p(y, z|\theta) = \sum_{i}^{n} \left[z_i \log\left(\lambda \mathcal{N}_1\right) + (1 - z_i) \log\left((1 - \lambda)\mathcal{N}_2\right)\right]$$

$$= \sum_{i} \left[z_i \log(\lambda) + z_i \log \mathcal{N}_1 + (1 - z_i) \log(1 - \lambda) + (1 - z_i) \log \mathcal{N}_2\right]$$

Two-part Gaussian mixture model

Missing data density is

$$p(z|y,\theta) = \frac{p(y,z|\theta)}{p(y,\theta)} \propto p(y,z|\theta)$$

$$= Bernoulli\left(\frac{\lambda\mathcal{N}(y|\mu_1,\sigma_1^2)}{\lambda\mathcal{N}(y|\mu_1,\sigma_1^2)+(1-\lambda)\mathcal{N}(y|\mu_2,\sigma_2^2)}\right)$$

This allows us to define $E[z_i|y_i,\theta] := \pi_i$ which will be used in find $Q(\theta|\theta_0)$ in the E-step

Two-part Gaussian mixture model

Next, **E-Step**! Construct $Q()$ function

$$
\begin{aligned}
Q(\theta|\theta_0) &= E_z\left[\log p(y, z|\theta)|y, \theta_0\right] \\
&= E\left(\sum_i^n \left[z_i \log\left(\lambda \mathcal{N}_1\right) + (1 - z_i)\log\left((1-\lambda)\mathcal{N}_2\right)\right]\right) \\
&= \sum_i^n \left[E(z_i)\log\left(\lambda \mathcal{N}_1\right) + E(1 - z_i)\log\left((1-\lambda)\mathcal{N}_2\right)\right] \\
&= \sum_i^n \left[\pi_i \log\left(\lambda \mathcal{N}_1\right) + (1 - \pi_i)\log\left((1-\lambda)\mathcal{N}_2\right)\right]
\end{aligned}
$$

Need current estimates of $\mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \lambda$ - Also, compute $E[z_i|y_i, \theta] := \pi_i$

Two-part Gaussian mixture model

M-Step! Maximize Q to get current estimates of $\mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \lambda$.

$$\hat{\mu}_1 = \frac{\sum_i \pi_i y_i}{\sum_i \pi_i} \tag{1}$$

$$\hat{\mu}_2 = \frac{\sum_i (1 - \pi_i) y_i}{\sum_i (1 - \pi_i)} \tag{2}$$

$$\hat{\sigma}_1^2 = \frac{\sum_i \pi_i (y_i - \mu_1)^2}{\sum_i \pi_i} \tag{3}$$

$$\hat{\sigma}_2^2 = \frac{\sum_i (1 - \pi_i)(y_i - \mu_2)^2}{\sum_i (1 - \pi_i)} \tag{4}$$

$$\hat{\lambda} = \frac{1}{n} \sum_i \pi_i \tag{5}$$

Two-part Gaussian mixture model

Class exercise: finish implementing this algorithm in R by doing first lab problem. Starter code is provided in the file `EM_GMM.R`

Canonical examples

- Two-part Gaussian mixture model
- Censored exponential data
  - Survival analysis, survival times exponentially distributed
  - Substantial right censoring
    - For censored individuals, true survival time is unknown

Censored exponential data

Suppose we have survival times $t_1, \dots, t_n \sim Exponential(\lambda)$.

- Do not observe all survival times because some are censored at times $c_1, \dots, c_n$.
- Actually observe $y_1, \dots, y_n$, where $y_i = min(t_i, c_i)$
  - Also have an indicator δ_i where $\delta_i = 1$ is $t_i \leq c_i$
    - i.e. $\delta_i = 1$ if not censored and $\delta_i = 0$ if censored

Censored exponential data

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- What is $p(y, z|\theta)$, the complete data density? - What is z?

Censored exponential data

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Asymptotic properties of MLEs

If it converges to the global maximum, EM finds the **MLE** of your likelihood function. This means that theory about MLEs holds for EM parameter estimates. Specifically:

- **Consistency**: Let the sequence of MLEs of θ_0 be denoted by $\hat{\theta}_n$. For any fixed $\epsilon > 0$, as $n \to \infty$

$$P(|\hat{\theta}_n - \theta_0| > \epsilon) \to 0$$

- Ensures estimate converges in probability to the true value
- **Asymptotic efficiency**: $\hat{\theta}$ achieves minimum variance among all asymptotically unbiased estimators

Asymptotic properties of MLEs

If it converges to the global maximum, EM finds the **MLE** of your likelihood function. This means that theory about MLEs holds for EM parameter estimates. Specifically:

- **Asymptotic Normality**: Let the sequence of MLEs of θ_0 be denoted by $\hat{\theta}_n$.

$$\sqrt{n}(\hat{\theta}_n - \theta_0) \to^d N(0, \sigma^2)$$

- A properly centered and scaled sequence is distributed normally with 0 mean and variance σ^2 as $n \to \infty$

Invariance Property of MLEs

Allows us to find the MLE of transformations of an MLE

- If $\hat{\theta}$ is the MLE of θ, then for any function $\tau(\hat{\theta})$ is the MLE of $\tau(\theta)$!

Invariance Property of MLEs

Suppose $Y_1, Y_2, \ldots, Y_n$ is a sample of independent Normal $N(\mu, \sigma^2)$ random variables with $E(Y_i) = \mu$.

- Sample mean $\hat{\mu} = \bar{Y} = \frac{1}{n}\sum_{i=1}^{n} Y_i$ is the MLE of μ

What is the MLE of $1/\mu$? Using invariance property of MLEs,

- $1/\hat{\mu} = 1/\bar{Y}$ is the MLE of $1/\mu$

Final thoughts

- *Ascent property of EM* is what guarantees stability via monotonically increasing likelihood
- Example of a minorization approach
  - Instead of maximizing the log-likelihood directly, which is difficult to evaluate, the algorithm constructs a minorizing function and optimizes that function instead

Resources

- good notes
- exercises in EM