3.4 - 3.5 Monte Carlo approaches to EM

Motivation

1. In the mean score approach, the MLE can be found by solving

$$E\left\{S_{\text{com}}(\eta) \mid \mathbf{y}_{\text{obs}}, \boldsymbol{\delta}\right\} = 0$$

which requires the knowledge of the conditional distribution of $\mathbf{y}_{\text{mis}}$ given $\mathbf{y}_{\text{obs}}$ and $\boldsymbol{\delta}$.

2. In the EM algorithm defined by
   - [E-step] Compute

$$Q\left(\eta \mid \eta^{(t)}\right) = E\left\{\ln L_{\text{com}}(\eta) \mid \mathbf{y}_{\text{obs}}, \boldsymbol{\delta}, \eta^{(t)}\right\}$$

   - [M-step] Find $\eta^{(t+1)}$ that maximizes $Q\left(\eta \mid \eta^{(t)}\right)$,

E-step is computationally cumbersome because it involves integral.

Monte Carlo EM (MCEM) method (Wei and Tanner, 1990)

In the E-step, first draw

$$\mathbf{y}_{\mathrm{mis}}^{*(1)}, \cdots, \mathbf{y}_{\mathrm{mis}}^{*(m)} \overset{iid}{\sim} p\left(\mathbf{y}_{\mathrm{mis}} \mid \mathbf{y}_{\mathrm{obs}}, \boldsymbol{\delta}, \eta^{(t)}\right) = \frac{f(\mathbf{y}, \boldsymbol{\delta}; \eta^{(t)})}{\int f(\mathbf{y}, \boldsymbol{\delta}; \eta^{(t)}) d\mathbf{y}_{\mathrm{mis}}}$$

and approximate

$$Q\left(\eta \mid \eta^{(t)}\right) \cong \frac{1}{m} \sum_{j=1}^{m} \ln f\left(\mathbf{y}_{\mathrm{obs}}, \mathbf{y}_{\mathrm{mis}}^{*(j)}, \boldsymbol{\delta}; \eta\right).$$

Example 3.14 (Nonignorable missing)

$$y_i \sim f\left(y_i \mid x_i; \theta\right)$$

Assume that x_i is always observed but we observe y_i only when $\delta_i = 1$ where $\delta_i \sim Bernoulli\left[\pi_i\left(\phi\right)\right]$ and

$$\pi_i\left(\phi\right) = \frac{\exp\left(\phi_0 + \phi_1 x_i + \phi_2 y_i\right)}{1 + \exp\left(\phi_0 + \phi_1 x_i + \phi_2 y_i\right)}.$$

To implement the MCEM method, we need to generate samples from

$$f\left(y_i \mid x_i, \delta_i = 0; \hat{\theta}, \hat{\phi}\right) = \frac{f\left(y_i \mid x_i; \hat{\theta}\right)\left[1 - \pi_i\left(\hat{\phi}\right)\right]}{\int f\left(y_i \mid x_i; \hat{\theta}\right)\left[1 - \pi_i\left(\hat{\phi}\right)\right] dy_i} \tag{1}$$

How to generate samples from (1)?

Rejection sampling method

Problem

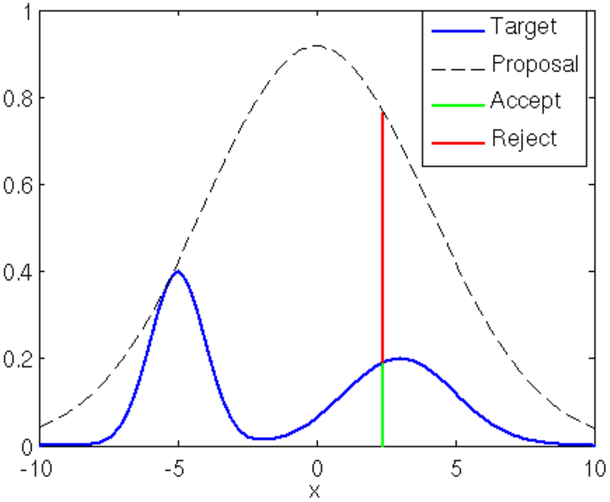
- Given a density of interest f, suppose that there exist a density g and a constant M such that
$$f(x) \leq Mg(x)$$
on the support of f.
- We are interested in generating samples from f, which is difficult. But, generating samples from g is easy.

Rejection sampling method

The rejection sampling method (or accept-rejection method) is

1. Sample $Y \sim g$ and $U \sim Unif\,(0,1)$.
2. Reject Y if
$$U > \frac{f\,(Y)}{Mg\,(Y)}.$$
In this case, do not record the value of Y as an element in the target random sample. Instead, return to step 1.
3. Otherwise, keep the value of Y. Set $X = Y$, and consider X to be an element of the target random sample.

Rejection sampling method



Remark

1. In the rejection sampling method,

$$\begin{aligned} P(Y \le y) &= P\left[X \le y \mid U \le \frac{f(X)}{Mg(X)}\right] \\ &= \frac{\int_{-\infty}^{y} \int_{0}^{f(x)/Mg(x)} du g(x)\, dx}{\int_{-\infty}^{\infty} \int_{0}^{f(x)/Mg(x)} du g(x)\, dx} \\ &= \frac{\int_{-\infty}^{y} f(x)\, dx}{\int_{-\infty}^{\infty} f(x)\, dx} \end{aligned}$$

2. The rejection sampling method can be applicable when the density f is known up to a multiplicative factor.

Example 3.14 (Cont'd)

We can use the following rejection method to generate m Monte Carlo samples from $f(y_i \mid x_i, \delta_i = 0; \hat{\theta}, \hat{\phi})$:

1. Generate y_i^* from $f(y_i \mid x_i; \hat{\theta})$.
2. Using y_i^*, compute

$$\pi_i^*\left(\hat{\phi}\right) = \frac{\exp\left(\hat{\phi}_0 + \hat{\phi}_1 x_i + \hat{\phi}_2 y_i^*\right)}{1 + \exp\left(\hat{\phi}_0 + \hat{\phi}_1 x_i + \hat{\phi}_2 y_i^*\right)}.$$

3. Accept y_i^* with probability $1 - \pi_i^*(\hat{\phi})$. Otherwise, goto Step 1.

Example 3.14 (Cont'd)

M-step: Update the parameters by solving

$$\sum_{i=1}^{n}\sum_{j=1}^{m} S\left(\theta; x_i, y_i^{*(j)}\right) = 0$$

and

$$\sum_{i=1}^{n}\sum_{j=1}^{m}\left\{\delta_i - \pi(\phi; x_i, y_i^{*(j)})\right\}\left(1, x_i, y_i^{*(j)}\right) = 0,$$

where $S(\theta; x_i, y_i) = \partial \log f(y_i \mid x_i; \theta)/\partial\theta$.

Importance sampling

Write $\theta \equiv \int h(x) f(x) dx = \int h(x) \frac{f(x)}{g(x)} g(x) dx$ for some density $g(x)$ and approximate θ by

$$\hat{\theta} = \sum_{i=1}^{n} w_i h(X_i)$$

where

$$w_i = \frac{f(X_i) / g(X_i)}{\sum_{j=1}^{n} f(X_j) / g(X_j)}$$

and $X_1, \cdots, X_n$ are IID with pdf $g(x)$. The weight w_i is called important weight.

(Details are skipped. Will be covered again in Chapter 6)

Markov Chain Monte Carlo (MCMC) method

What is MCMC ?

- Markov Chain Monte Carlo: A body of methods for generating pseudorandom draws from probability distributions via Markov chains
- Markov chain: A sequence of random variables in which the distribution of each element depends only the previous one:

$$\{X_t; t = 1, 2, \cdots\}$$

  where

$$P\left(X_t \mid X_0, X_1, \cdots, X_{t-1}\right) = P\left(X_t \mid X_{t-1}\right).$$

- "Today is the tomorrow of yesterday".

History of MCMC

1. Metropolis et al (1953): algorithm for indirect simulation of energy distributions
2. Hastings (1970): extension of Metropolis to a non-symmetric jumping distributions
3. Geman and Geman (1984): the “Gibbs sampler” for Bayesian image reconstruction
4. Tanner and Wong (1987): data augmentation for Bayesian inference in generic missing-data problems
5. Gelfand and Smith (1990): simulation of marginal distributions by repeated draws from conditionals

Basic setup for MCMC

- X: generic random vector with density $f(X)$
- $f(X)$: difficult to simulate directly
- Goal: construct a Markov chain $\left\{X^{(t)}; t = 1, 2 \cdots\right\}$ with f as its stationary distribution,

$$P\left(X^{(t)}\right) \rightarrow f \quad \text{as } t \rightarrow \infty$$

or

$$\frac{1}{N}\sum_{t=1}^{N} h\left(X^{(t)}\right) \rightarrow E_f\left[h(X)\right] = \int h(x) f(x)\, dx \tag{2}$$

as $N \rightarrow \infty$.

- A Markov chain that satisfies (2) is called ergodic.

Metropolis-Hastings algorithm: Algorithm

Starting with $X^{(0)}$ iterate for $t = 1, 2, \cdots$

1. Draw $X^* \sim q\left(\cdot \mid X^{(t-1)}\right)$.
2. Compute
$$R\left(X^*, X^{(t-1)}\right) = \frac{q\left(X^{(t-1)} \mid X^*\right)}{q\left(X^* \mid X^{(t-1)}\right)} \frac{f\left(X^*\right)}{f\left(X^{(t-1)}\right)}$$
and
$$\rho\left(X^*, X^{(t-1)}\right) = \min\{R\left(X^*, X^{(t-1)}\right), 1\}.$$
3. With probability $\rho\left(X^*, X^{(t-1)}\right)$ set $X^{(t)} = X^*$. Otherwise set $X^{(t)} = X^{(t-1)}$.

Remark

- The probability of acceptance does not depend on the normalization constant: If $f(x) = C \cdot \pi(x)$, then

$$R\left(X^* \mid X^{(t-1)}\right) = \frac{q\left(X^{(t-1)} \mid X^*\right)}{q\left(X^* \mid X^{(t-1)}\right)} \frac{\pi\left(X^*\right)}{\pi\left(X^{(t-1)}\right)}.$$

- Usually, q is chosen so that $q\left(y \mid x\right)$ is easy to sample from.
- The Markov chain is irreducible if $q(X \mid X^{(t-1)}) > 0$ for all $X, X^{(t-1)} \in \operatorname{supp}(f)$: every state can be reached in a single step.

Remark (Cont'd)

- In the independent chain where $q(X^* \mid X^{(t)}) = q(X^*)$, the Metropolis-Hastings ratio is

$$R\left(X^*, X^{(t)}\right) = \frac{f\left(X^*\right)/q\left(X^*\right)}{f\left(X^{(t)}\right)/q\left(X^{(t)}\right)},$$

  which is the ratio of the importance weight for X^* over the importance weight for $X^{(t)}$. Thus, the Metropolis-Hastings ratio $R\left(X^*, X^{(t)}\right)$ is also called the importance ratio.
- The basic idea of the MH algorithm is
  - from the current position x, move to y according to $q\left(y \mid x\right)$ and
  - we decide to stay at y, roughly speaking, with probability $f\left(y\right)/f\left(x\right)$.
- Hence, $q\left(y \mid x\right)$ having more mass when $f\left(y\right)$ is larger is a good candidate.

Example 3.14 (Normal-Cauchy model)

- Let $Y_1, \cdots, Y_n \overset{iid}{\sim} N(\theta, 1)$
- Prior: Cauchy distribution

$$\pi(\theta) = \frac{1}{\pi(1+\theta^2)} \tag{3}$$

- Posterior

$$\begin{aligned} \pi(\theta \mid y) &\propto exp\left\{-\frac{\sum_{i=1}^{n}(y_i-\theta)^2}{2}\right\} \times \frac{1}{1+\theta^2} \\ &\propto exp\left\{-\frac{n(\theta-\bar{y})^2}{2}\right\} \times \frac{1}{1+\theta^2} \end{aligned}$$

- We want to generate $\theta \sim \pi(\theta \mid y)$.

Example 3.13 (Normal-Cauchy model)

- MH algorithm
  1. Generate θ^* from Cauchy (0,1).
  2. Given $y_1, \cdots, y_n$, compute the importance ratio

  $$R\left(\theta^*, \theta^{(t)}\right) = \frac{\pi(\theta^* \mid y)/\pi(\theta^*)}{\pi(\theta^{(t)} \mid y)/\pi(\theta^{(t)})} = \frac{f\left(y \mid \theta^*\right)}{f\left(y \mid \theta^{(t)}\right)}$$

     where $f(y \mid \theta) = C \exp\left\{-n\left(\theta - \bar{y}\right)^2/2\right\}$ and $\pi(\theta)$ is defined in (3).
  3. Accept θ^* as $\theta^{(t+1)}$ with probability $\rho(\theta^{(t)}, \theta^*) = \min\left\{R\left(\theta^{(t)}, \theta^*\right), 1\right\}$.

Random-walk Metropolis: Idea

- In the Metropolis-Hastings algorithm the proposal is from $X \sim q\left(\cdot \mid X^{(t-1)}\right)$.
- A popular choice for the proposal is $q(X \mid X^{(t-1)}) = g(X - X^{(t-1)})$ with g being a symmetric distribution. That is,

$$X = X^{(t-1)} + \epsilon, \quad \epsilon \sim g.$$

- The Metropolis-Hastings ratio becomes

$$R\left(X^*, X^{(t)}\right) = \frac{g\left(X^{(t-1)} - X^*\right)}{g\left(X^* - X^{(t-1)}\right)} \frac{f\left(X^*\right)}{f\left(X^{(t-1)}\right)} = \frac{f\left(X^*\right)}{f\left(X^{(t-1)}\right)}.$$

- We accept
    - every move to a more probable state with probability 1.
    - Moves to less probable states with a probability $f(X^*)/f(X^{(t-1)}) < 1$.

Example 3.18 (GLMM)

- Basic Setup: Let y_{ij} be a binary random variable (that takes 0 or 1) with probability $p_{ij} = Pr\left(y_{ij} = 1 \mid \mathbf{x}_{ij}, a_i\right)$ and we assume that

$$\text{logit}\left(p_{ij}\right) = \mathbf{x}_{ij}'\boldsymbol{\beta} + a_i$$

where $\mathbf{x}_{ij}$ is a p-dimensional covariate associate with j-th repetition of unit i, $\boldsymbol{\beta}$ is the parameter of interest that can represent the treatment effect due to $\mathbf{x}$, and a_i represents the random effect associate with unit i. We assume that a_i are iid with $N\left(0, \sigma^2\right)$.

- Missing data : a_i
- Observed likelihood:

$$L_{\text{obs}}\left(\boldsymbol{\beta}, \sigma^2\right) = \prod_i \int \left\{ \prod_j p(\mathbf{x}_{ij}, a_i; \boldsymbol{\beta})^{y_{ij}} \left[1 - p(x_{ij}, a_i; \boldsymbol{\beta})\right]^{1-y_{ij}} \right\} \frac{1}{\sigma} \phi\left(\frac{a_i}{\sigma}\right) d a_i$$

where $\phi(\cdot)$ is the pdf of the standard normal distribution.

- To apply EM algorithm, note that a_i are observed in the complete sample log-likelihood

$$\ell_{\text{com}}(\beta, \sigma^2) = \ell_{\text{com},1}(\beta) + \ell_{\text{com},2}(\sigma^2)$$

where

$$\ell_{\text{com},1}(\beta) = \sum_i \sum_j \left[y_{ij} \log p_{ij}(\beta) + (1 - y_{ij}) \log\{1 - p_{ij}(\beta)\} \right]$$

and

$$\ell_{\text{com},2}(\sigma^2) = -\frac{1}{2} \log\left(2\pi\sigma^2\right) - \frac{1}{2\sigma^2} a_i^2$$

- Thus, in the E-step, we need to compute

$$Q(\theta \mid \theta^{(t)}) = E\left\{ \ell_{\text{com}}(\beta, \sigma^2) \mid \text{data}, \theta^{(t)} \right\}$$

where the conditional expectation is with respect to $f(a_i \mid \mathbf{x}_i, \mathbf{y}_i; \theta^{(t)})$.

- MCEM approach: Target distribution is

$$f(a_i \mid \mathbf{x}_i, \mathbf{y}_i; \hat{\boldsymbol{\beta}}, \hat{\sigma}) \propto f_1(\mathbf{y}_i \mid \mathbf{x}_i, a_i; \hat{\boldsymbol{\beta}}) f_2\left(a_i; \hat{\sigma}\right).$$

- M-H algorithm 1: Generate a_i^* from $f_2\left(a_i; \hat{\sigma}\right)$. Then, we accept a_i^* with probability

$$\rho\left(a_i^*, a_i^{(t-1)}\right) = \min\left\{\frac{f_1\left(\mathbf{y}_i \mid \mathbf{x}_i, a_i^*; \hat{\boldsymbol{\beta}}\right)}{f_1\left(\mathbf{y}_i \mid \mathbf{x}_i, a_i^{(t-1)}; \hat{\boldsymbol{\beta}}\right)}, 1\right\}.$$

M-H algorithm 2: Random Walk Metropolis algorithm

1. Starting with any $a_i^{(0)}$, iterate for $t = 1, 2 \cdots$
2. Draw $\epsilon_i \sim N(0, 0.1)$ and set
$$a_i^* = a_i^{(t-1)} + \epsilon_i$$
3. Compute
$$R(a_i^*, a_i^{(t-1)}) = \frac{f(a_i^* \mid \mathbf{x}_i, \mathbf{y}_i; \hat{\boldsymbol{\beta}}, \hat{\sigma})}{f(a_i^{(t-1)} \mid \mathbf{x}_i, \mathbf{y}_i; \hat{\boldsymbol{\beta}}, \hat{\sigma})}$$
and
$$\rho(a_i^*, a_i^{(t-1)}) = \min\{R(a_i^*, a_i^{(t+1)}), 1\}.$$
4. Set $a_i^{(t)} = a_i^*$ with probability $\rho(a_i^*, a_i^{(t+1)})$. Otherwise, set $a_i^{(t)} = a_i^{(t-1)}$.

Summary

- Monte Carlo methods can be used to compute the E-step of the EM algorithm.
- Sometimes, MCMC algorithm is used for the E-step and so it is an MCMC-EM algorithm.
- Because of the nature of MC algorithm, the convergence is not guaranteed for a fixed MC sample size. Booth and Hobert (1999) discussed some convergence criteria for MCEM.

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