Modern Computational Statistics

Lecture 11: Advanced EM

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- While EM increases the marginal likelihood in each iteration and often converges to a stationary point, we are not clear about the convergence rate and how does that relate to the missing data scenario.
- Moreover, the requirements of tractable conditional distribution and easy complete data MLE may be too restrictive in practice.
- In this lecture, we will discuss the convergence theory for EM and introduce some variants of it that can be applied in more general settings.

Example: Censored Survival Times

- Recall that in the censored survival times example, given the observed data $Y = \{(t_1, \delta_1), \ldots, (t_n, \delta_n)\}$, where t_j follows an exponential distribution with mean μ and can be either censored or not as indicated by δ_j.
- Assume $\delta_i = 0, i \leq r,\ \delta_i = 1, i > r$. The MLE of μ is $\hat{\mu} = \sum_{i=1}^{n} t_i / r$
- EM update formula

$$\mu^{(k+1)} = \frac{\sum_{i=1}^{n} t_i + (n-r)\mu^{(k)}}{n}$$

- Therefore,

$$\mu^{(k+1)} - \hat{\mu} = \frac{n-r}{n}(\mu^{(k)} - \hat{\mu})$$

Linear convergence, rate depends on the amount of missing information

We can view EM update as a map

$$\theta^{(t+1)} = \Phi(\theta^{(t)}), \quad \Phi(\theta) = \arg\max_{\theta'} Q(\theta'|\theta)$$

where $Q(\theta'|\theta) = \mathbb{E}_{p(z|x,\theta)} \log p(x, z|\theta')$

Lemma 1

If for some θ^*, $\mathcal{L}(\theta^*) \geq \mathcal{L}(\theta)$, $\forall\theta$, then for every EM algorithm

$$\mathcal{L}(\Phi(\theta^*)) = \mathcal{L}(\theta^*), \; Q(\Phi(\theta^*)|\theta^*) = Q(\theta^*|\theta^*)$$

and

$$p(z|x, \Phi(\theta^*)) = p(z|x, \theta^*), \text{ a.s.}$$

Lemma 2

If for some θ^*, $\mathcal{L}(\theta^*) > \mathcal{L}(\theta)$, $\forall \theta \neq \theta^*$, then for every EM algorithm

$$\Phi(\theta^*) = \theta^*$$

Theorem 1

Suppose that $\theta^{(t)}, t = 0, 1, \ldots$ is an instance of an EM algorithm such that

- the sequence $\mathcal{L}(\theta^{(t)})$ is bounded
- for some $\lambda > 0$ and all t,

$$Q(\theta^{(t+1)}|\theta^{(t)}) - Q(\theta^{(t)}|\theta^{(t)}) \geq \lambda(\theta^{(t+1)} - \theta^{(t)})(\theta^{(t+1)} - \theta^{(t)})^T$$

Then the sequence $\theta^{(t)}$ converges to some θ^*

- Since $\theta^{(t+1)} = \Phi(\theta^{(t)})$ maximizes $Q(\theta'|\theta^{(t)})$, we have

$$\frac{\partial Q}{\partial \theta'}(\theta^{(t+1)}|\theta^{(t)}) = 0$$

- For all t, there exists a $0 \leq \alpha_0^{(t+1)} \leq 1$ such that

$$Q(\theta^{(t+1)}|\theta^{(t)}) - Q(\theta^{(t)}|\theta^{(t)}) = -(\theta^{(t+1)} - \theta^{(t)}) \cdot \frac{\partial^2 Q}{\partial \theta'^2}(\theta_0^{(t+1)}|\theta^{(t)})(\theta^{(t+1)} - \theta^{(t)})^T$$

  where $\theta_0^{(t+1)} = \alpha_0 \theta^{(t)} + (1 - \alpha_0)\theta^{(t+1)}$

- If the sequence $\frac{\partial^2 Q}{\partial \theta'^2}(\theta_0^{(t+1)}|\theta^{(t)})$ is negative definite with eigenvalues bounded away from zero and $\mathcal{L}(\theta^{(t)})$ is bounded, by Theorem 1, $\theta^{(t)}$ converges to some θ^*

- When EM converges, it converges to a fixed point of the map

$$\theta^* = \Phi(\theta^*)$$

- Taylor expansion of Φ at θ^* yields

$$\theta^{(t+1)} - \theta^* = \Phi(\theta^{(t)}) - \Phi(\theta^*) \approx \nabla\Phi(\theta^*)(\theta^{(t)} - \theta^*)$$

- The global rate of EM defined as

$$\rho = \lim_{t\to\infty} \frac{\|\theta^{(t+1)} - \theta^*\|}{\|\theta^{(t)} - \theta^*\|}$$

equals the largest eigenvalue of $\nabla\Phi(\theta^*)$ and $\rho < 1$ when the observed Fisher information $-\nabla^2\mathcal{L}(\theta^*)$ is positive definite.

- As aforementioned, $\Phi(\theta)$ maximize $Q(\theta'|\theta)$, therefore

$$\frac{\partial Q}{\partial \theta'}(\Phi(\theta)|\theta) = 0, \quad \forall \theta$$

- Differentiate w.r.t. θ

$$\frac{\partial^2 Q}{\partial \theta'^2}(\Phi(\theta)|\theta)\nabla\Phi(\theta) + \frac{\partial^2 Q}{\partial \theta \partial \theta'}(\Phi(\theta)|\theta) = 0$$

let $\theta = \theta^*$

$$\nabla\Phi(\theta^*) = \left(-\frac{\partial^2 Q}{\partial \theta'^2}(\theta^*|\theta^*)\right)^{-1} \frac{\partial^2 Q}{\partial \theta \partial \theta'}(\theta^*|\theta^*) \qquad (1)$$

- If $\frac{\partial^2 Q}{\partial \theta'^2}(\theta^{(t+1)}|\theta^{(t)})$ is negative definite with eigenvalues bounded away from zero, then

$$-\frac{\partial^2 Q}{\partial \theta'^2}(\theta^*|\theta^*) = \mathbb{E}_{p(z|x,\theta^*)}\left(-\nabla^2 \log p(x,z|\theta^*)\right)$$

  is positive definite, known as the **complete information**

- The marginal log-likelihood can be rewritten as

$$\begin{aligned}\mathcal{L}(\theta') &= \mathbb{E}_{p(z|x,\theta)} \log p(x,z|\theta') - \mathbb{E}_{p(z|x,\theta)} \log p(z|x,\theta) \\ &= Q(\theta'|\theta) - H(\theta'|\theta)\end{aligned}$$

  Therefore

$$\frac{\partial^2 Q}{\partial \theta \partial \theta'}(\theta'|\theta) = \frac{\partial^2 H}{\partial \theta \partial \theta'}(\theta'|\theta)$$

- Some properties of $H(\theta|\theta) = \mathbb{E}_{p(z|x,\theta)} \log p(z|x,\theta)$

$$\frac{\partial H}{\partial \theta'}(\theta|\theta) = 0$$
$$\frac{\partial^2 H}{\partial \theta \partial \theta'}(\theta|\theta) = -\frac{\partial^2 H}{\partial \theta'^2}(\theta|\theta)$$

- Therefore,

$$\frac{\partial^2 Q}{\partial \theta \partial \theta'}(\theta^*|\theta^*) = \frac{\partial^2 H}{\partial \theta \partial \theta'}(\theta^*|\theta^*) = -\frac{\partial^2 H}{\partial \theta'^2}(\theta^*|\theta^*)$$

is positive semidefinite (variance of the score $\nabla \log p(z|x,\theta^*)$), known as the **missing information**

$$\mathcal{L}(\theta') = Q(\theta'|\theta) - H(\theta'|\theta)$$

- Differentiate both side w.r.t. θ' twice

$$\nabla^2\mathcal{L}(\theta') = \frac{\partial^2 Q}{\partial\theta'^2}(\theta'|\theta) - \frac{\partial^2 H}{\partial\theta'^2}(\theta'|\theta)$$

- The *missing-information principle*

$$\underbrace{-\frac{\partial^2 Q}{\partial\theta'^2}(\theta|\theta)}_{I_{\text{complete}}} = \underbrace{-\nabla^2\mathcal{L}(\theta)}_{I_{\text{observed}}} + \underbrace{-\frac{\partial^2 H}{\partial\theta'^2}(\theta|\theta)}_{I_{\text{missing}}}$$

- Substitute in (1)

$$\begin{aligned}\nabla\Phi(\theta^*) &= I^{-1}_{\text{complete}}(\theta^*) I_{\text{missing}}(\theta^*) \\ &= \left(I_{\text{observed}}(\theta^*) + I_{\text{missing}}(\theta^*)\right)^{-1} I_{\text{missing}}(\theta^*)\end{aligned}$$

- When $I_{\text{observed}} = -\nabla^2 \mathcal{L}(\theta^*)$ is positive definite, the eigenvalues of $\nabla \Phi(\theta^*)$ are all less than 1, EM has a linear convergence rate.
- The rate of convergence depends on the relative size of $I_{\text{observed}}(\theta^*)$ and $I_{\text{missing}}(\theta^*)$. EM converges rapidly when the missing information is small.
- The fraction of information loss may vary across different component of θ, so some component may converge faster than other components.
- See Wu (1983) for more detailed discussions.

EM for Maximum A Posterior

- EM can be easily modified for the Maximum A Posterior (MAP) estimate instead of the MLE.
- Suppose the log-prior penalty term is $R(\theta)$. We only have to maximize

$$Q(\theta|\theta^{(t)}) + R(\theta) \tag{2}$$

  in the M-step
- Monotonicity.

$$\begin{aligned}\mathcal{L}(\theta^{(t+1)}) + R(\theta^{(t+1)}) &\geq \mathcal{F}(\theta^{(t+1)}|\theta^{(t)}) + R(\theta^{(t+1)}) \\ &\geq \mathcal{F}(\theta^{(t)}|\theta^{(t)}) + R(\theta^{(t)}) \\ &= \mathcal{L}(\theta^{(t)}) + R(\theta^{(t)})\end{aligned}$$

- If $R(\theta)$ corresponds to conjugate prior, (2) can be maximized in the same manner as $Q(\theta|\theta^{(t)})$.

- The E-step requires finding the expected complete data log-likelihood $Q(\theta|\theta^{(t)})$. When this expectation is difficult to compute, we can approximate it via Monte Carlo methods
- **Monte Carlo EM** (Wei and Tanner, 1990)
  - Draw missing data $z_1^{(t)}, \ldots, z_m^{(t)}$ from the conditional distribution $p(z|x, \theta^{(t)})$
  - Compute a Monte Carlo estimate of $Q(\theta|\theta^{(t)})$

$$\hat{Q}^{(t+1)}(\theta|\theta^{(t)}) = \frac{1}{m}\sum_{i=1}^{m} \log p(x, z_i^{(t)}|\theta)$$

  - Update $\theta^{(t+1)}$ to maximize $\hat{Q}^{(t+1)}(\theta|\theta^{(t)})$.

Remark: It is recommended to let m changes along iterations (small at the beginning and increases as iterations progress)

Example: Censored Survival Times

- By the lack of memory, it is easy to compute the expected complete data log-likelihood, which lead to the ordinary EM update

$$\mu_{\text{EM}}^{(k+1)} = \frac{\sum_{i=1}^{n} t_i + (n-r)\mu^{(k)}}{n}$$

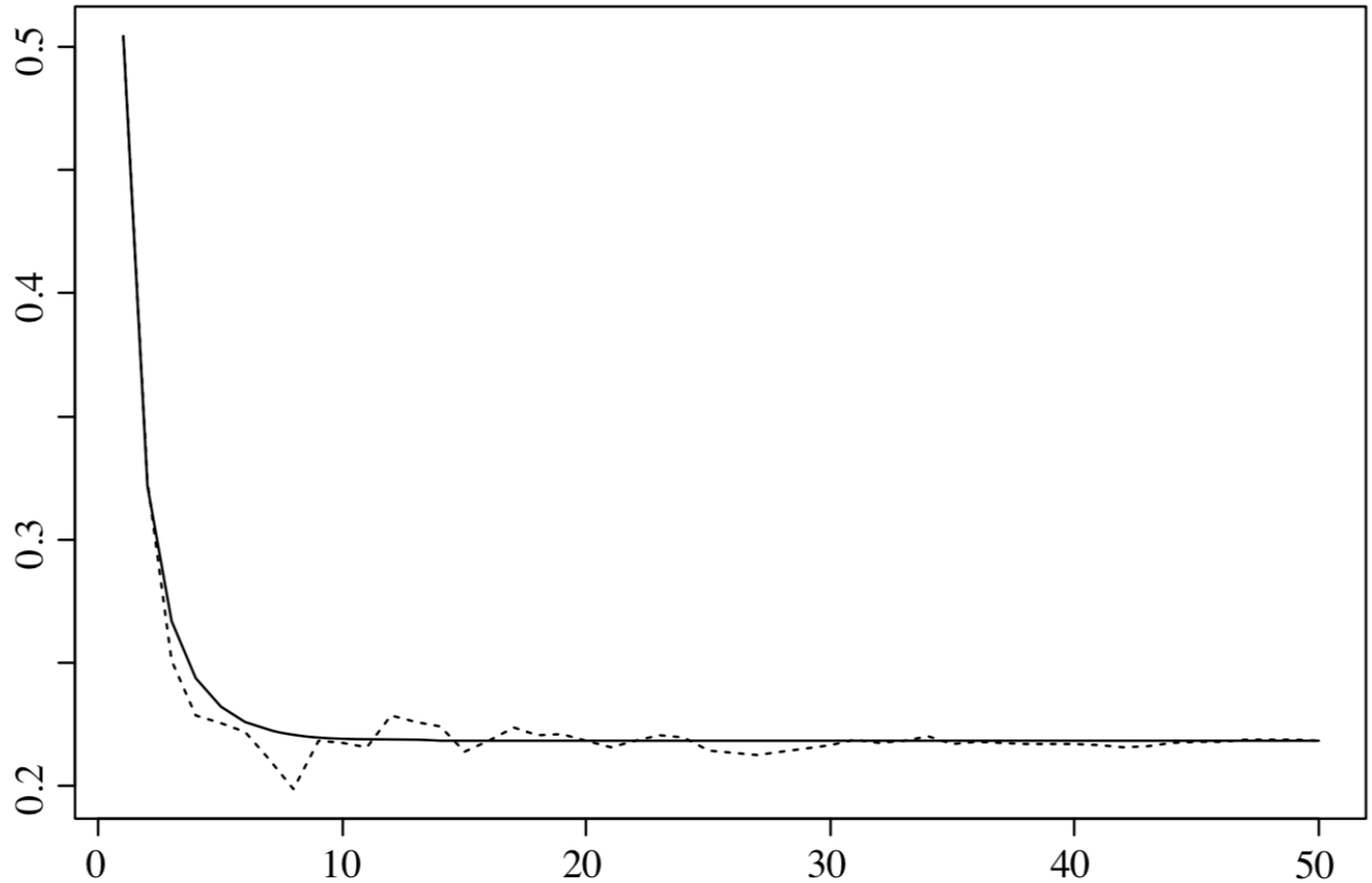
- In MCEM, we can sample from the conditional distribution

$$\boldsymbol{T}_j = (T_{j,r+1}, \ldots, T_{j,n}),\ T_{j,l} - t_l \sim \text{Exp}(\mu^{(k)}), \quad l = r+1, \ldots, n$$

for $j = 1, \ldots, m^{(k)}$, and the update formula is

$$\mu_{\text{MCEM}}^{(k+1)} = \frac{\sum_{i=1}^{n} t_i + \frac{1}{m^{(k)}} \sum_{j=1}^{m^{(k)}} \boldsymbol{T}_j^T \mathbf{1}}{n}$$

Examples: Censored Survival Times



Improving the M-step

- One of the appeals of the EM algorithm is that $Q(\theta|\theta^{(t)})$ is often simpler to maximize than the marginal likelihood
- In some cases, however, the M-step cannot be carried out easily even though the computation of $Q(\theta|\theta^{(t)})$ is straightforward in the E-step
- For such situations, Dempster et al (1977) defined a generalized EM algorithm (GEM) for which the M-step only requires $\theta^{(t+1)}$ to improve $Q(\theta|\theta^{(t)})$

$$Q(\theta^{(t+1)}|\theta^{(t)}) \geq Q(\theta^{(t+1)}|\theta^{(t)})$$

- We can easily show that GEM is also monotonic in $\mathcal{L}$

$$\mathcal{L}(\theta^{(t+1)}) \geq \mathcal{F}(q^{(t)}, \theta^{(t+1)}) \geq \mathcal{F}(q^{(t)}, \theta^{(t)}) = \mathcal{L}(\theta^{(t)})$$

- Meng and Rubin (1993) replaces the M-step with a series of computationally cheaper conditional maximization (CM) steps, leading to the **ECM** algorithm
- The M-step in ECM contains a collection of simple CM steps, called a CM *cycle*. For $s = 1, \ldots, S$, the s-th CM step requires the maximization of $Q(\theta|\theta^{(t)})$ subject to a constraint

$$\theta^{(t+s/S)} = \arg\max_{\theta} Q(\theta|\theta^{(t)}), \quad \text{s.t. } g_s(\theta) = g_s(\theta^{(t+(s-1)/S)})$$

- The efficiency of ECM depends on the choice of constraints. Examples: Blockwise updates (coordinate ascent).
- One may also insert an E-step between each pair of CM-steps, updating Q at every stage of the CM cycle.

- Suppose we have n independent observations from the following k-variate normal model

$$Y_i \sim \mathcal{N}(X_i\beta, \Sigma), \quad i = 1, \ldots, n$$

  - $X_i \in \mathbb{R}^{k\times p}$ is a known design matrix for the i-th observation
  - β is a vector of p unknown parameters
  - Σ is a $d \times d$ unknown variance-covariance matrix
- The complete data log-likelihood (up to a constant) is

$$L(\beta, \Sigma|Y) = -\frac{n}{2}\log|\Sigma| - \frac{1}{2}\sum_{i=1}^{n}(Y_i - X_i\beta)^T\Sigma^{-1}(Y_i - X_i\beta)$$

- Generally, MLE does not has closed form solution except in special cases (e.g., $\Sigma = \sigma^2 I$)

A Coordinate Ascent Algorithm

- Although the joint maximization of β and Σ are not generally in closed form, a coordinate ascent algorithm does exist
- Given $\Sigma = \Sigma^{(t)}$, the conditional MLE of β is simply the weighted least-square estimate

$$\beta^{(t+1)} = \left(\sum_{i=1}^{n} X_i^T (\Sigma^{(t)})^{-1} X_i \right)^{-1} \left(\sum_{i=1}^{n} X_i^T (\Sigma^{(t)})^{-1} Y_i \right)$$

- Given $\beta = \beta^{(t+1)}$, the conditional MLE of Σ is the cross-product of the residuals

$$\Sigma^{(t+1)} = \frac{1}{n} \sum_{i=1}^{n} (Y_i - X_i \beta^{(t+1)})(Y_i - X_i \beta^{(t+1)})^T$$

- Now suppose that we also have missing data

$$Y_i \sim \mathcal{N}(X_i\beta, \Sigma), \quad i = n+1, \ldots, m$$

for which only the design matrix $X_i,\ i > n$ are known

- The complete data log-likelihood

$$L(\beta, \Sigma|Y) = -\frac{m}{2}\log|\Sigma| - \frac{1}{2}\sum_{i=1}^{m}(Y_i - X_i\beta)^T\Sigma^{-1}(Y_i - X_i\beta)$$

- Expected values of sufficient statistics observed data and current parameter $\theta^{(t)} = (\beta^{(t)}, \Sigma^{(t)})$

$$\mathbb{E}(Y_i|Y_{\text{obs}}, \theta^{(t)}) = X_i\beta^{(t)}$$
$$\mathbb{E}(Y_iY_i^T|Y_{\text{obs}}, \theta^{(t)}) = \Sigma^{(t)} + (X_i\beta^{(t)})(X_i\beta^{(t)})^T$$

Expected complete-data log-likelihood

$$
\begin{aligned}
Q(\theta|\theta^{(t)}) &= -\frac{m}{2}\log|\Sigma| - \frac{1}{2}\sum_{i=1}^{n}(Y_i - X_i\beta)^T\Sigma^{-1}(Y_i - X_i\beta) \\
&\quad - \frac{1}{2}\sum_{i=n+1}^{m}\mathbb{E}\left((Y_i - X_i\beta)^T\Sigma^{-1}(Y_i - X_i\beta)\right) \\
&= -\frac{m}{2}\log|\Sigma| - \frac{1}{2}\sum_{i=1}^{n}(Y_i - X_i\beta)^T\Sigma^{-1}(Y_i - X_i\beta) \\
&\quad - \frac{1}{2}\sum_{i=n+1}^{m}(\mathbb{E}Y_i - X_i\beta)^T\Sigma^{-1}(\mathbb{E}Y_i - X_i\beta) + C
\end{aligned}
$$

where $C = \frac{1}{2}\sum_{i=n+1}^{m}\mathbb{E}(Y_i)^T\Sigma^{-1}\mathbb{E}(Y_i) - \mathbb{E}(Y_i^T\Sigma^{-1}Y_i)$ is a constant independent of the parameter β.

CM-steps: Update β

- The first CM-step, maximize Q given $\Sigma = \Sigma^{(t)}$.
- Since C is independent of β, we can maximize

$$-\frac{m}{2}\log|\Sigma| - \frac{1}{2}\sum_{i=1}^{n}(Y_i - X_i\beta)^T\Sigma^{-1}(Y_i - X_i\beta)$$
$$-\frac{1}{2}\sum_{i=n+1}^{m}(\mathbb{E}Y_i - X_i\beta)^T\Sigma^{-1}(\mathbb{E}Y_i - X_i\beta)$$

$$\Rightarrow \beta^{(t+1)} = \left(\sum_{i=1}^{m} X_i^T\Sigma^{(t)}X_i\right)^{-1}\left(\sum_{i=1}^{m} X_i^T\Sigma^{(t)}\hat{Y}_i\right)$$

where

$$\hat{Y}_i = \begin{cases} Y_i, & i \le n \\ X_i\beta^{(t)}, & i > n \end{cases}$$

CM-steps: Update Σ

- The second CM-step, maximize Q with $\beta = \beta^{(t+1)}$
- Rewrite Q as

$$Q(\theta|\theta^{(t)}) = \frac{m}{2}\log|\Sigma^{-1}| - \frac{1}{2}\sum_{i=1}^{n}\mathrm{Tr}\left(\Sigma^{-1}(Y_i - X_i\beta)(Y_i - X_i\beta)^T\right) - \frac{1}{2}\sum_{i=n+1}^{m}\mathrm{Tr}\left(\Sigma^{-1}\mathbb{E}\left((Y_i - X_i\beta)(Y_i - X_i\beta)^T\right)\right)$$

- Similarly as in the complete data case

$$\Sigma^{(t+1)} = \frac{1}{m}\left(\sum_{i=1}^{n}(Y_i - X_i\beta^{(t+1)})(Y_i - X_i\beta^{(t+1)})^T + \sum_{i=n+1}^{m}\Sigma^{(t)} + \sum_{i=n+1}^{m}X_i(\beta^{(t)} - \beta^{(t+1)})(\beta^{(t)} - \beta^{(t+1)})^T X_i^T\right)$$

- Both the E-step and the two CM-steps can be implemented using close form solutions, no numerical iteration required.
- Both CM-steps improves Q

$$\begin{aligned} Q(\beta^{(t+1)}, \Sigma^{(t+1)} | \beta^{(t)}, \Sigma^{(t)}) &\geq Q(\beta^{(t+1)}, \Sigma^{(t)} | \beta^{(t)}, \Sigma^{(t)}) \\ &\geq Q(\beta^{(t)}, \Sigma^{(t)} | \beta^{(t)}, \Sigma^{(t)}) \end{aligned}$$

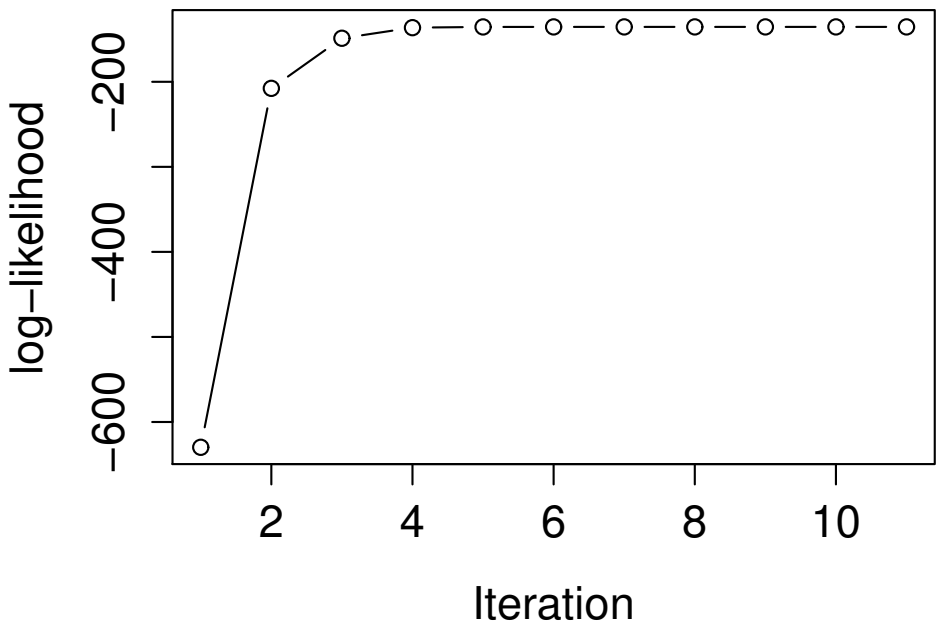
- ECM in this case can be viewed as an efficient generalization of iterative reweighted least squares, in the presence of missing data.

Example: A Simulation Study

We generate 120 design matrices at random and simulate 100 observations with $\beta = \begin{pmatrix} 2 \\ 1 \end{pmatrix}$, $\Sigma = \begin{pmatrix} 1, & 0.1 \\ 0.1 & 2 \end{pmatrix}$

ECM estimates

$$\hat{\beta} = \begin{pmatrix} 2.068 \\ 1.087 \end{pmatrix}, \quad \hat{\Sigma} = \begin{pmatrix} 0.951 & 0.214 \\ 0.214 & 2.186 \end{pmatrix}$$



EM Gradient Algorithm

- Iterative optimization can be considered when direct maximization is not available.
- All numerical optimization can apply and that would yield an algorithm that has nested iterative loops (e.g., ECM inserts conditional maximization steps within each CM cycle)
- To avoid the computational burden of nested looping, Lange proposed to use one single step of Newton's method

$$\begin{aligned}\theta^{(t+1)} &= \theta^{(t)} - \left(\frac{\partial^2 Q}{\partial \theta'^2}(\theta^{(t)}|\theta^{(t)})\right)^{-1} \frac{\partial Q}{\partial \theta'}(\theta^{(t)}|\theta^{(t)}) \\ &= \theta^{(t)} - \left(\frac{\partial^2 Q}{\partial \theta'^2}(\theta^{(t)}|\theta^{(t)})\right)^{-1} \nabla \mathcal{L}(\theta^{(t)})\end{aligned}$$

- This EM gradient algorithm has the same rate of convergence as the full EM algorithm.

- When EM is slow, we can use the relatively simple analytic setup from EM to motivate particular forms for Newton-like steps.
- **Aitken Acceleration**. Newton update

$$\theta^{(t+1)} = \theta^{(t)} - (\nabla^2 \mathcal{L}(\theta^{(t)}))^{-1} \nabla \mathcal{L}(\theta^{(t)}) \tag{3}$$

Note that $\nabla \mathcal{L}(\theta^{(t)}) = \frac{\partial Q}{\partial \theta'}(\theta^{(t)}|\theta^{(t)})$ and

$$0 = \frac{\partial Q}{\partial \theta'}(\theta_{\text{EM}}^{(t+1)}|\theta^{(t)}) \approx \frac{\partial Q}{\partial \theta'}(\theta^{(t)}|\theta^{(t)}) + \frac{\partial^2 Q}{\partial \theta'^2}(\theta^{(t)}|\theta^{(t)})(\theta_{\text{EM}}^{(t+1)} - \theta^{(t)})$$

substitute in (3)

$$\theta^{(t+1)} = \theta^{(t)} + (I_{\text{observed}}(\theta^{(t)}))^{-1} I_{\text{complete}}(\theta^{(t)})(\theta_{\text{EM}}^{(t+1)} - \theta^{(t)})$$

- Many other acceleration exists (e.g., Quasi-Newton methods).

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