## Statistics 580

## The EM Algorithm

## Introduction

The EM algorithm is a very general iterative algorithm for parameter estimation by maximum likelihood when some of the random variables involved are not observed i.e., considered missing or incomplete. The EM algorithm formalizes an intuitive idea for obtaining parameter estimates when some of the data are missing:
i. replace missing values by estimated values,
ii. estimate parameters.
iii. Repeat

- step (i) using estimated parameter values as true values, and
- step (ii) using estimated values as "observed" values, iterating until convergence.

This idea has been in use for many years before Orchard and Woodbury (1972) in their missing information principle provided the theoretical foundation of the underlying idea. The term EM was introduced in Dempster, Laird, and Rubin (1977) where proof of general results about the behavior of the algorithm was first given as well as a large number of applications.

For this discussion, let us suppose that we have a random vector $\mathbf{y}$ whose joint density $f(\mathbf{y} ; \boldsymbol{\theta})$ is indexed by a $p$-dimensional parameter $\boldsymbol{\theta} \in \Theta \subseteq R^{p}$. If the complete-data vector $\mathbf{y}$ were observed, it is of interest to compute the maximum likelihood estimate of $\boldsymbol{\theta}$ based on the distribution of $\mathbf{y}$. The $\log$-likelihood function of $\mathbf{y}$

$$
\log L(\boldsymbol{\theta} ; \mathbf{y})=\ell(\boldsymbol{\theta} ; \mathbf{y})=\log f(\mathbf{y} ; \boldsymbol{\theta})
$$

is then required to be maximized.
In the presence of missing data, however, only a function of the complete-data vector $\mathbf{y}$, is observed. We will denote this by expressing $\mathbf{y}$ as $\left(\mathbf{y}_{\text {obs }}, \mathbf{y}_{\text {mis }}\right)$, where $\mathbf{y}_{\text {obs }}$ denotes the observed but "incomplete" data and $\mathbf{y}_{\text {mis }}$ denotes the unobserved or "missing" data. For simplicity of description, assume that the missing data are missing at random (Rubin, 1976), so that

$$
\begin{aligned}
f(\mathbf{y} ; \boldsymbol{\theta}) & =f\left(\mathbf{y}_{\text {obs }}, \mathbf{y}_{\text {mis }} ; \boldsymbol{\theta}\right) \\
& =f_{1}\left(\mathbf{y}_{\text {obs }} ; \boldsymbol{\theta}\right) \cdot f_{2}\left(\mathbf{y}_{\text {mis }} \mid \mathbf{y}_{\text {obs }} ; \boldsymbol{\theta}\right),
\end{aligned}
$$

where $f_{1}$ is the joint density of $\mathbf{y}_{\text {obs }}$ and $f_{2}$ is the joint density of $\mathbf{y}_{\text {mis }}$ given the observed data $\mathbf{y}_{\text {obs }}$, respectively. Thus it follows that

$$
\ell_{\text {obs }}\left(\boldsymbol{\theta} ; \mathbf{y}_{\text {obs }}\right)=\ell(\boldsymbol{\theta} ; \mathbf{y})-\log f_{2}\left(\mathbf{y}_{\text {mis }} \mid \mathbf{y}_{\text {obs }} ; \boldsymbol{\theta}\right),
$$

where $\ell_{\text {obs }}\left(\boldsymbol{\theta} ; \mathbf{y}_{\text {obs }}\right)$ is the observed-data log-likelihood.

EM algorithm is useful when maximizing $\ell_{\text {obs }}$ can be difficult but maximizing the completedata $\log$-likelihood $\ell$ is simple. However, since $\mathbf{y}$ is not observed, $\ell$ cannot be evaluated and hence maximized. The EM algorithm attempts to maximize $\ell(\boldsymbol{\theta} ; \mathbf{y})$ iteratively, by replacing it by its conditional expectation given the observed data $\mathbf{y}_{\text {obs }}$. This expectation is computed with respect to the distribution of the complete-data evaluated at the current estimate of $\boldsymbol{\theta}$. More specifically, if $\boldsymbol{\theta}^{(0)}$ is an initial value for $\boldsymbol{\theta}$, then on the first iteration it is required to compute

$$
Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(0)}\right)=E_{\boldsymbol{\theta}^{(0)}}\left[\ell(\boldsymbol{\theta} ; \mathbf{y}) \mid \mathbf{y}_{\text {obs }}\right] .
$$

$Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(0)}\right)$ is now maximized with respect to $\boldsymbol{\theta}$, that is, $\boldsymbol{\theta}^{(1)}$ is found such that

$$
Q\left(\boldsymbol{\theta}^{(1)} ; \boldsymbol{\theta}^{(0)}\right) \geq Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(0)}\right)
$$

for all $\boldsymbol{\theta} \in \Theta$. Thus the EM algorithm consists of an E-step (Estimation step) followed by an M-step (Maximization step) defined as follows:

E-step: Compute $Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)$ where

$$
Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)=E_{\boldsymbol{\theta}^{(t)}}\left[\ell(\boldsymbol{\theta} ; \mathbf{y}) \mid \mathbf{y}_{\text {obs }}\right]
$$

M-step: Find $\boldsymbol{\theta}^{(t+1)}$ in $\Theta$ such that

$$
Q\left(\boldsymbol{\theta}^{(t+1)} ; \boldsymbol{\theta}^{(t)}\right) \geq Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)
$$

for all $\boldsymbol{\theta} \in \Theta$.
The E-step and the M-step are repeated alternately until the difference $L\left(\boldsymbol{\theta}^{(t+1)}\right)-L\left(\boldsymbol{\theta}^{(t)}\right)$ is less than $\delta$, where $\delta$ is a prescribed small quantity.

The computation of these two steps simplify a great deal when it can be shown that the $\log$-likelihood is linear in the sufficient statistic for $\boldsymbol{\theta}$. In particular, this turns out to be the case when the distribution of the complete-data vector (i.e., $\mathbf{y}$ ) belongs to the exponential family. In this case, the E-step reduces to computing the expectation of the completedata sufficient statistic given the observed data. When the complete-data are from the exponential family, the M-step also simplifies. The M-step involves maximizing the expected log-likelihood computed in the E-step. In the exponential family case, actually maximizing the expected log-likelihood to obtain the next iterate can be avoided. Instead, the conditional expectations of the sufficient statistics computed in the E-step can be directly substituted for the sufficient statistics that occur in the expressions obtained for the complete-data maximum likelihood estimators of $\boldsymbol{\theta}$, to obtain the next iterate. Several examples are discussed below to illustrate these steps in the exponential family case.

As a general algorithm available for complex maximum likelihood computations, the EM algorithm has several appealing properties relative to other iterative algorithms such as Newton-Raphson. First, it is typically easily implemented because it relies on completedata computations: the E-step of each iteration only involves taking expectations over complete-data conditional distributions. The M -step of each iteration only requires completedata maximum likelihood estimation, for which simple closed form expressions are already
available. Secondly, it is numerically stable: each iteration is required to increase the loglikelihood $\ell\left(\boldsymbol{\theta} ; \mathbf{y}_{\text {obs }}\right)$ in each iteration, and if $\ell\left(\boldsymbol{\theta} ; \mathbf{y}_{\text {obs }}\right)$ is bounded, the sequence $\ell\left(\boldsymbol{\theta}^{(t)} ; \mathbf{y}_{\text {obs }}\right)$ converges to a stationery value. If the sequence $\boldsymbol{\theta}^{(t)}$ converges, it does so to a local maximum or saddle point of $\ell\left(\boldsymbol{\theta} ; \mathbf{y}_{\text {obs }}\right)$ and to the unique MLE if $\ell\left(\boldsymbol{\theta} ; \mathbf{y}_{\text {obs }}\right)$ is unimodal. A disadvantage of EM is that its rate of convergence can be extremely slow if a lot of data are missing: Dempster, Laird, and Rubin (1977) show that convergence is linear with rate proportional to the fraction of information about $\boldsymbol{\theta}$ in $\ell(\boldsymbol{\theta} ; \mathbf{y})$ that is observed.

## Example 1: Univariate Normal Sample

Let the complete-data vector $\mathbf{y}=\left(y_{1}, \ldots, y_{n}\right)^{T}$ be a random sample from $N\left(\mu, \sigma^{2}\right)$. Then

$$
\begin{aligned}
f\left(\mathbf{y} ; \mu, \sigma^{2}\right) & =\left(\frac{1}{2 \pi \sigma^{2}}\right)^{n / 2} \exp \left\{-\frac{1}{2} \sum_{i=1}^{n} \frac{\left(y_{i}-\mu\right)^{2}}{\sigma^{2}}\right\} \\
& =\left(\frac{1}{2 \pi \sigma^{2}}\right)^{n / 2} \exp \left\{-1 / 2 \sigma^{2}\left(\sum y_{i}^{2}-2 \mu \sum y_{i}+n \mu^{2}\right)\right\}
\end{aligned}
$$

which implies that $\left(\sum y_{i}, \sum y_{i}^{2}\right)$ are sufficient statistics for $\boldsymbol{\theta}=\left(\mu, \sigma^{2}\right)^{T}$. The complete-data log-likelihood function is:

$$
\begin{aligned}
\ell\left(\mu, \sigma^{2} ; \mathbf{y}\right) & =-\frac{n}{2} \log \left(\sigma^{2}\right)-\frac{1}{2} \sum_{i=1}^{n} \frac{\left(y_{i}-\mu\right)^{2}}{\sigma^{2}}+\text { constant } \\
& =-\frac{n}{2} \log \left(\sigma^{2}\right)-\frac{1}{2 \sigma^{2}} \sum_{i=1}^{n} y_{i}^{2}+\frac{\mu}{\sigma^{2}} \sum_{i=1}^{n} y_{i}-\frac{n \mu^{2}}{\sigma^{2}}+\text { constant }
\end{aligned}
$$

It follows that the log-likelihood based on complete-data is linear in complete-data sufficient statistics. Suppose $y_{i}, i=1, \ldots, m$ are observed and $y_{i}, i=m+1, \ldots, n$ are missing (at random) where $y_{i}$ are assumed to be i.i.d. $N\left(\mu, \sigma^{2}\right)$. Denote the observed data vector by $\left.\mathbf{y}_{\text {obs }}=\left(y_{1}, \ldots, y_{m}\right)^{T}\right)$. Since the complete-data $\mathbf{y}$ is from the exponential family, the E-step requires the computation of

$$
E_{\boldsymbol{\theta}}\left(\sum_{i=1}^{n} y_{i} \mid \mathbf{y}_{\text {obs }}\right) \text { and } E_{\boldsymbol{\theta}}\left(\sum_{i=1}^{N} y_{i}^{2} \mid \mathbf{y}_{\text {obs }}\right),
$$

instead of computing the expectation of the complete-data log-likelihood function shown above. Thus, at the $t^{\text {th }}$ iteration of the E-step, compute

$$
\begin{align*}
s_{1}^{(t)} & =E_{\mu^{(t)}, \sigma^{2(t)}}\left(\sum_{i=1}^{n} y_{i} \mid \mathbf{y}_{\text {obs }}\right)  \tag{1}\\
& =\sum_{i=1}^{m} y_{i}+(n-m) \mu^{(t)}
\end{align*}
$$

since $E_{\mu^{(t)}, \sigma^{2(t)}}\left(y_{i}\right)=\mu^{(t)}$ where $\mu^{(t)}$ and $\sigma^{2^{(t)}}$ are the current estimates of $\mu$ and $\sigma^{2}$, and

$$
\begin{align*}
s_{2}^{(t)} & =E_{\mu^{(t), \sigma^{2}(t)}}\left(\sum_{i=1}^{n} y_{i}^{2} \mid \mathbf{y}_{\mathrm{obs}}\right)  \tag{2}\\
& =\sum_{i=1}^{m} y_{i}^{2}+(n-m)\left[\sigma^{(t)^{2}}+\mu^{(t)^{2}}\right]
\end{align*}
$$

since $E_{\mu^{(t), \sigma^{2}}}\left(y_{i}^{2}\right)=\sigma^{2^{(t)}}+\mu^{(t)^{2}}$.
For the M-step, first note that the complete-data maximum likelihood estimates of $\mu$ and $\sigma^{2}$ are:

$$
\hat{\mu}=\frac{\sum_{i=1}^{n} y_{i}}{n} \text { and } \hat{\sigma}^{2}=\frac{\sum_{i=1}^{n} y_{i}^{2}}{n}-\left(\frac{\sum_{i=1}^{n} y_{i}}{n}\right)^{2}
$$

The M -step is defined by substituting the expectations computed in the E-step for the complete-data sufficient statistics on the right-hand side of the above expressions to obtain expressions for the new iterates of $\mu$ and $\sigma^{2}$. Note that complete-data sufficient statistics themselves cannot be computed directly since $y_{m+1}, \ldots, y_{n}$ have not been observed. We get the expressions

$$
\begin{equation*}
\mu^{(t+1)}=\frac{s_{1}^{(t)}}{n} \tag{3}
\end{equation*}
$$

and

$$
\begin{equation*}
\sigma^{2^{(t+1)}}=\frac{s_{2}^{(t)}}{n}-\mu^{(t+1)^{2}} \tag{4}
\end{equation*}
$$

Thus, the E-step involves computing evaluating (1) and (2) beginning with starting values $\mu^{(0)}$ and $\sigma^{2^{(0)}}$. M-step involves substituting these in (3) and (4) to calculate new values $\mu^{(1)}$ and $\sigma^{2^{(1)}}$, etc. Thus, the EM algorithm iterates successively between (1) and (2) and (3) and (4). Of course, in this example, it is not necessary to use of EM algorithm since the maximum likelihood estimates for $\left(\mu, \sigma^{2}\right)$ are clearly given by $\hat{\mu}=\sum_{i=1}^{m} y_{i} / m$ and $\hat{\sigma}^{2}=\sum_{i=1}^{m} y_{i}^{2} / m-\hat{\mu}^{2} \square$.

## Example 2: Sampling from a Multinomial population

In the Example 1, "incomplete data" in effect was "missing data" in the conventional sense. However, in general, the EM algorithm applies to situations where the complete data may contain variables that are not observable by definition. In that set-up, the observed data can be viewed as some function or mapping from the space of the complete data.

The following example is used by Dempster, Laird and Rubin (1977) as an illustration of the EM algorithm. Let $\mathbf{y}_{\text {obs }}=(38,34,125)^{T}$ be observed counts from a multinomial population with probabilities: $\left(\frac{1}{2}-\frac{1}{2} \theta, \frac{1}{4} \theta, \frac{1}{2}+\frac{1}{4} \theta\right)$. The objective is to obtain the maximum likelihood estimate of $\theta$. First, to put this into the framework of an incomplete data problem, define $\mathbf{y}=\left(y_{1}, y_{2}, y_{3}, y_{4}\right)^{T}$ with multinomial probabilities $\left(\frac{1}{2}-\frac{1}{2} \theta, \frac{1}{4} \theta, \frac{1}{4} \theta, \frac{1}{2}\right) \equiv\left(p_{1}, p_{2}, p_{3}, p_{4}\right)$.

The $\mathbf{y}$ vector is considered complete-data. Then define $\mathbf{y}_{\text {obs }}=\left(y_{1}, y_{2}, y_{3}+y_{4}\right)^{T}$. as the observed data vector, which is a function of the complete-data vector. Since only $y_{3}+y_{4}$ is observed and $y_{3}$ and $y_{4}$ are not, the observed data is considered incomplete. However, this is not simply a missing data problem.

The complete-data log-likelihood is

$$
\ell(\theta ; \mathbf{y})=y_{1} \log p_{1}+y_{2} \log p_{2}+y_{3} \log p_{3}+y_{4} \log p_{4}+\text { const. }
$$

which is linear in $y_{1}, y_{2}, y_{3}$ and $y_{4}$ which are also the sufficient statistics. The E-step requires that $E_{\theta}\left(\mathbf{y} \mid \mathbf{y}_{\text {obs }}\right)$ be computed; that is compute

$$
\begin{aligned}
& E_{\theta}\left(y_{1} \mid \mathbf{y}_{\text {obs }}\right)=y_{1}=38 \\
& E_{\theta}\left(y_{2} \mid \mathbf{y}_{\text {obs }}\right)=y_{2}=34 \\
& E_{\theta}\left(y_{3} \mid \mathbf{y}_{\text {obs }}\right)=E_{\theta}\left(y_{3} \mid y_{3}+y_{4}\right)=125\left(\frac{1}{4} \theta\right) /\left(\frac{1}{2}+\frac{1}{4} \theta\right)
\end{aligned}
$$

since, conditional on $\left(y_{3}+y_{4}\right), y_{3}$ is distributed as $\operatorname{Binomial}(125, p)$ where

$$
p=\frac{\frac{1}{4} \theta}{\frac{1}{2}+\frac{1}{4} \theta}
$$

Similarly,

$$
E_{\theta}\left(y_{4} \mid \mathbf{y}_{\mathrm{obs}}\right)=E_{\theta}\left(y_{4} \mid y_{3}+y_{4}\right)=125\left(\frac{1}{2}\right) /\left(\frac{1}{2}+\frac{1}{4} \theta\right)
$$

which is similar to computing $E_{\theta}\left(y_{3} \mid \mathbf{y}_{\text {obs }}\right)$. But only

$$
\begin{equation*}
y_{3}^{(t)}=E_{\theta^{(t)}}\left(y_{3} \mid \mathbf{y}_{\mathrm{obs}}\right)=\frac{125\left(\frac{1}{4}\right) \theta^{(t)}}{\left(\frac{1}{2}+\frac{1}{4} \theta^{(t)}\right)} \tag{1}
\end{equation*}
$$

needs to be computed at the $t^{\text {th }}$ iteration of the E-step as seen below.
For the M-step, note that the complete-data maximum likelihood estimate of $\theta$ is

$$
\frac{y_{2}+y_{3}}{y_{1}+y_{2}+y_{3}}
$$

(Note: Maximize

$$
\ell(\theta ; \mathbf{y})=y_{1} \log \left(\frac{1}{2}-\frac{1}{2} \theta\right)+y_{2} \log \frac{1}{4} \theta+y_{3} \log \frac{1}{4} \theta+y_{4} \log \frac{1}{2}
$$

and show that the above indeed is the maximum likelihood estimate of $\theta$ ). Thus, substitute the expectations from the E-step for the sufficient statistics in the expression for maximum likelihood estimate $\theta$ above to get

$$
\begin{equation*}
\theta^{(t+1)}=\frac{34+y_{3}^{(t)}}{72+y_{3}^{(t)}} \tag{2}
\end{equation*}
$$

Iterations between (1) and (2) define the EM algorithm for this problem. The following table shows the convergence results of applying EM to this problem with $\theta^{(0)}=0.50$.

Table 1. The EM Algorithm for Example 2 (from Little and Rubin (1987))

| $t$ | $\theta^{(t)}$ | $\theta^{(t)}-\hat{\theta}$ | $\left(\theta^{(t+1)}-\hat{\theta}\right) /\left(\theta^{(t)}-\hat{\theta}\right)$ |
| :---: | :---: | :---: | :---: |
| 0 | 0.500000000 | 0.126821498 | 0.1465 |
| 1 | 0.608247423 | 0.018574075 | 0.1346 |
| 2 | 0.624321051 | 0.002500447 | 0.1330 |
| 3 | 0.626488879 | 0.000332619 | 0.1328 |
| 4 | 0.626777323 | 0.000044176 | 0.1328 |
| 5 | 0.626815632 | 0.000005866 | 0.1328 |
| 6 | 0.626820719 | 0.000000779 | $\cdot$ |
| 7 | 0.626821395 | 0.000000104 | $\cdot$ |
| 8 | 0.626821484 | 0.000000014 | $\cdot$ |

## Example 3: Sample from Binomial/ Poisson Mixture

The following table shows the number of children of N widows entitled to support from a certain pension fund.

$$
\begin{array}{llllllll}
\text { Number of Children: } & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\
\text { Observed \# of Widows: } & n_{0} & n_{1} & n_{2} & n_{3} & n_{4} & n_{5} & n_{6}
\end{array}
$$

Since the actual data were not consistent with being a random sample from a Poisson distribution (the number of widows with no children being too large) the following alternative model was adopted. Assume that the discrete random variable is distributed as a mixture of two populations, thus:

Population A: with probability $\xi$, the random
variable takes the value 0 , and
Mixture of Populations:
Population B: with probability $(1-\xi)$, the random variable follows a Poisson with mean $\lambda$
Let the observed vector of counts be $\mathbf{n}_{\text {obs }}=\left(n_{0}, n_{1}, \ldots, n_{6}\right)^{T}$. The problem is to obtain the maximum likelihood estimate of $(\lambda, \xi)$. This is reformulated as an incomplete data problem by regarding the observed number of widows with no children be the sum of observations that come from each of the above two populations.
Define

$$
\begin{aligned}
n_{0} & =n_{A}+n_{B} \\
n_{A} & =\# \text { widows with no children from population } \mathrm{A} \\
n_{B} & =n_{o}-n_{A}=\# \text { widows with no children from population } \mathrm{B}
\end{aligned}
$$

Now, the problem becomes an incomplete data problem because $n_{A}$ is not observed. Let $\mathbf{n}=\left(n_{A}, n_{B}, n_{1}, n_{2}, \ldots, n_{6}\right)$ be the complete-data vector where we assume that $n_{A}$ and $n_{B}$ are observed and $n_{0}=n_{A}+n_{B}$.

Then

$$
\begin{aligned}
f(\mathbf{n} ; \xi, \lambda) & =k(\mathbf{n})\left\{P\left(y_{0}=0\right)\right\}^{n_{0}} \Pi_{i=1}^{\infty}\left\{P\left(y_{i}=i\right)\right\}^{n_{i}} \\
& =k(\mathbf{n})\left[\xi+(1-\xi) e^{-\lambda}\right]^{n_{0}}\left[\Pi_{i=1}^{6}\left\{(1-\xi) \frac{e^{-\lambda} \lambda^{i}}{i!}\right\}^{n_{i}}\right] \\
& =k(\mathbf{n})\left[\xi+(1-\xi) e^{-\lambda}\right]^{n_{A}+n_{B}}\left\{(1-\xi) e^{-\lambda}\right\}^{\sum_{i=1}^{6} n_{i}}\left[\Pi_{i=1}^{6}\left(\frac{\lambda^{i}}{i!}\right)^{n_{i}}\right]
\end{aligned}
$$

where $k(\mathbf{n})=\sum_{i=1}^{6} n_{i} / n_{0}!n_{1}!\ldots n_{6}!$. Obviously, the complete-data sufficient statistic is $\left(n_{A}, n_{B}, n_{1}, n_{2}, \ldots, n_{6}\right)$. The complete-data log-likelihood is

$$
\begin{aligned}
\ell(\xi, \lambda ; \mathbf{n})= & n_{0} \log \left(\xi+(1-\xi) e^{-\lambda}\right) \\
& +\left(N-n_{0}\right)[\log (1-\xi)-\lambda]+\sum_{i=1}^{6} i n_{i} \log \lambda+\text { const } .
\end{aligned}
$$

Thus, the complete-data log-likelihood is linear in the sufficient statistic. The E-step requires the computing of

$$
E_{\xi, \lambda}\left(\mathbf{n} \mid \mathbf{n}_{\mathrm{obs}}\right)
$$

This computation results in

$$
E_{\xi, \lambda}\left(n_{i} \mid \mathbf{n}_{\mathrm{obs}}\right)=n_{i} \quad \text { for } \quad i=1, \ldots, 6
$$

and

$$
E_{\xi, \lambda}\left(n_{A} \mid \mathbf{n}_{\mathrm{obs}}\right)=\frac{n_{0} \xi}{\xi+(1-\xi) \exp (-\lambda)}
$$

since $n_{A}$ is $\operatorname{Binomial}\left(n_{0}, p\right)$ with $p=\frac{p_{A}}{p_{A}+p_{B}}$ where $p_{A}=\xi$ and $p_{B}=(1-\xi) e^{-\lambda}$. The expression for $E_{\xi, \lambda}\left(n_{B} \mid \mathbf{n}_{\text {obs }}\right)$ is equivalent to that for $E\left(n_{A}\right)$ and will not be needed for Estep computations. So the E-step consists of computing

$$
\begin{equation*}
n_{A}^{(t)}=\frac{n_{0} \xi^{(t)}}{\xi^{(t)}+\left(1-\xi^{(t)}\right) \exp \left(-\lambda^{(t)}\right)} \tag{1}
\end{equation*}
$$

at the $t^{t h}$ iteration.
For the M-step, the complete-data maximum likelihood estimate of $(\xi, \lambda)$ is needed. To obtain these, note that $n_{A} \sim \operatorname{Bin}(N, \xi)$ and that $n_{B}, n_{1}, \ldots, n_{6}$ are observed counts for $i=0,1, \ldots, 6$ of a Poisson distribution with parameter $\lambda$. Thus, the complete-data maximum likelihood estimate's of $\xi$ and $\lambda$ are

$$
\hat{\xi}=\frac{n_{A}}{N},
$$

and

$$
\hat{\lambda}=\sum_{i=1}^{6} \frac{i n_{i}}{n_{B}+\sum_{i=1}^{6} n_{i}} .
$$

The M-step computes

$$
\begin{equation*}
\xi^{(t+1)}=\frac{n_{A}^{(t)}}{N} \tag{2}
\end{equation*}
$$

and

$$
\begin{equation*}
\lambda^{(t+1)}=\sum_{i=1}^{6} \frac{i n_{i}}{n_{B}^{(t)}+\sum_{i=1}^{6} n_{i}} \tag{3}
\end{equation*}
$$

where $n_{B}^{(t)}=n_{0}-n_{A}^{(t)}$.
The EM algorithm consists of iterating between (1), and (2) and (3) successively. The following data are reproduced from Thisted(1988).

| Number of children | 0 | 1 | 2 | 3 | 4 | 5 | 6 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Number of widows | 3,062 | 587 | 284 | 103 | 33 | 4 | 2 |

Starting with $\xi^{(0)}=0.75$ and $\lambda^{(0)}=0.40$ the following results were obtained.

Table 2. EM Iterations for the Pension Data

| $t$ | $\xi$ | $\lambda$ | $n_{A}$ | $n_{B}$ |
| :--- | :--- | :--- | :---: | :---: |
| 0 | 0.75 | 0.40 | 2502.779 | 559.221 |
| 1 | 0.614179 | 1.035478 | 2503.591 | 558.409 |
| 2 | 0.614378 | 1.036013 | 2504.219 | 557.781 |
| 3 | 0.614532 | 1.036427 | 2504.704 | 557.296 |
| 4 | 0.614651 | 1.036747 | 2505.079 | 556.921 |
| 5 | 0.614743 | 1.036995 | 2505.369 | 556.631 |

A single iteration produced estimates that are within $0.5 \%$ of the maximum likelihood estimate's and are comparable to the results after about four iterations of Newton-Raphson. However, the convergence rate of the subsequent iterations are very slow; more typical of the behavior of the EM algorithm.

Example 4: Variance Component Estimation (Little and Rubin(1987))
The following example is from Snedecor and Cochran (1967, p.290). In a study of artificial insemination of cows, semen samples from six randomly selected bulls were tested for their ability to produce conceptions. The number of samples tested varied from bull to bull and the response variable was the percentage of conceptions obtained from each sample. Here the interest is on the variability of the bull effects which is assumed to be a random effect. The data are:

Table 3. Data for Example 4 (from Snedecor and Cochran(1967))

| Bull $(i)$ | Percentages of Conception | $n_{i}$ |
| :---: | :--- | :--- |
| 1 | $46,31,37,62,30$ | 5 |
| 2 | 70,59 | 2 |
| 3 | $52,44,57,40,67,64,70$ | 7 |
| 4 | $47,21,70,46,14$ | 5 |
| 5 | $42,64,50,69,77,81,87$ | 7 |
| 6 | $35,68,59,38,57,76,57,29,60$ | $\underline{9}$ |
| Total | $\mathbf{3 5}$ |  |

A common model used for analysis of such data is the oneway random effects model:

$$
y_{i j}=a_{i}+\epsilon_{i j}, \quad j=1, \ldots, n_{i}, \quad i=1, \ldots, k ;
$$

where it is assumed that the bull effects $a_{i}$ are distributed as i.i.d. $N\left(\mu, \sigma_{a}^{2}\right)$ and the withinbull effects (errors) $\epsilon_{i j}$ as i.i.d. $N\left(0, \sigma^{2}\right)$ random variables where $a_{i}$ and $\epsilon_{i j}$ are independent. The standard oneway random effects analysis of variance is:

| Source | d.f. | S.S. | M.S. | F | E(M.S.) |
| :--- | ---: | ---: | ---: | :---: | :---: |
| Bull | 5 | 3322.059 | 664.41 | 2.68 | $\sigma^{2}+5.67 \sigma_{a}^{2}$ |
| Error | 29 | 7200.341 | 248.29 |  | $\sigma^{2}$ |
| Total | 34 | 10522.400 |  |  |  |

Equating observed and expected mean squares from the above gives $s^{2}=248.29$ as the estimate of $\sigma^{2}$ and $(664.41-248.29) / 5.67=73.39$ as the estimate of $\sigma_{a}^{2}$.

To construct an EM algorithm to obtain MLE's of $\theta=\left(\mu, \sigma_{a}^{2}, \sigma^{2}\right)$, first consider the joint density of $\mathbf{y}^{*}=(\mathbf{y}, \mathbf{a})^{T}$ where $\mathbf{y}^{*}$ is assumed to be complete-data. This joint density can be written as a product of two factors: the part first corresponds to the joint density of $y_{i j}$ given $a_{i}$ and the second to the joint density of $a_{i}$.

$$
\begin{aligned}
f\left(\mathbf{y}^{*} ; \boldsymbol{\theta}\right) & =f_{1}(\mathbf{y} \mid \mathbf{a} ; \boldsymbol{\theta}) f_{2}(\mathbf{a} ; \boldsymbol{\theta}) \\
& =\Pi_{i} \Pi_{j}\left\{\frac{1}{\sqrt{2 \pi} \sigma} e^{-\frac{1}{2 \sigma^{2}}\left(y_{i j}-a_{i}\right)^{2}}\right\} \Pi_{i}\left\{\frac{1}{\sqrt{2 \pi} \sigma_{a}} e^{-\frac{1}{2 \sigma_{a}^{2}}\left(a_{i}-\mu\right)^{2}}\right\}
\end{aligned}
$$

Thus, the log-likelihood is linear in the following complete-data sufficient statistics:

$$
\begin{aligned}
& T_{1}=\sum a_{i} \\
& T_{2}=\sum_{i} a_{i}^{2} \\
& T_{3}=\sum_{i} \sum_{j}\left(y_{i j}-a_{i}\right)^{2}=\sum_{i} \sum_{j}\left(y_{i j}-\bar{y}_{i .}\right)^{2}+\sum_{i} n_{i}\left(\bar{y}_{i .}-a_{i}\right)^{2}
\end{aligned}
$$

Here complete-data assumes that both $\mathbf{y}$ and $\mathbf{a}$ are available. Since only $\mathbf{y}$ is observed, let $\mathbf{y}_{\text {obs }}^{*}$ $=\mathbf{y}$. Then the E-step of the EM algorithm requires the computation of the expectations of $T_{1}, T_{2}$ and $T_{3}$ given $\mathbf{y}_{\text {obs }}^{*}$, i.e., $E_{\boldsymbol{\theta}}\left(T_{i} \mid \mathbf{y}\right)$ for $i=1,2,3$. The conditional distribution of a given $\mathbf{y}$ is needed for computing these expectations. First, note that the joint distribution of $\mathbf{y}^{*}=$ $(\mathbf{y}, \mathbf{a})^{T}$ is $(N+k)$-dimensional multivariate normal: $N\left(\boldsymbol{\mu}^{*}, \Sigma^{*}\right)$ where $\boldsymbol{\mu}^{*}=\left(\boldsymbol{\mu}, \boldsymbol{\mu}_{a}\right)^{T}, \boldsymbol{\mu}=$ $\mu \mathbf{j}_{N}, \boldsymbol{\mu}_{a}=\mu \mathbf{j}_{k}$ and $\Sigma^{*}$ is the $(N+k) \times(N+k)$ matrix

$$
\Sigma^{*}=\left(\begin{array}{cc}
\Sigma & \Sigma_{12} \\
\Sigma_{12}^{T} & \sigma_{a}^{2} I
\end{array}\right)
$$

Here

$$
\Sigma=\left[\begin{array}{cccc}
\Sigma_{1} & & & 0 \\
& \Sigma_{2} & & \\
& & \ddots & \\
0 & & & \Sigma_{k}
\end{array}\right], \Sigma_{12}=\sigma_{a}^{2}\left[\begin{array}{cccc}
\mathbf{j}_{n_{1}} & & & 0 \\
& \mathbf{j}_{n_{2}} & & \\
& & \ddots & \\
0 & & & \mathbf{j}_{n_{k}}
\end{array}\right]
$$

where $\Sigma_{i}=\sigma^{2} I_{n_{i}}+\sigma_{a}^{2} J_{n_{i}}$ is an $n_{i} \times n_{i}$ matrix. The covariance matrix $\Sigma$ of the joint distribution of $\mathbf{y}$ is obtained by recognizing that the $y_{i j}$ are jointly normal with common mean $\mu$ and common variance $\sigma^{2}+\sigma_{a}^{2}$ and covariance $\sigma_{a}^{2}$ within the same bull and 0 between bulls. That is

$$
\begin{array}{rlr}
\operatorname{Cov}\left(y_{i j}, y_{i^{\prime} j^{\prime}}\right) & =\operatorname{Cov}\left(a_{i}+\epsilon_{i j}, a_{i^{\prime}}+\epsilon_{i^{\prime} j^{\prime}}\right) \\
& =\sigma^{2}+\sigma_{a}^{2} & \text { if } i=i^{\prime}, j=j^{\prime}, \\
& =\sigma_{a}^{2} & \text { if } i=i^{\prime}, j \neq j^{\prime}, \\
& =0 & \text { if } i \neq i^{\prime} .
\end{array}
$$

$\Sigma_{12}$ is covariance of $\mathbf{y}$ and $\mathbf{a}$ and follows from the fact that $\operatorname{Cov}\left(y_{i j}, a_{i}\right)=\sigma_{a}^{2}$ if $i=i^{\prime}$ and 0 if $i \neq i^{\prime}$. The inverse of $\Sigma$ is needed for computation of the conditional distribution of a given $\mathbf{y}$ and obtained as

$$
\Sigma^{-1}=\left[\begin{array}{lllc}
\Sigma_{1}^{-1} & & & 0 \\
& \Sigma_{2}^{-1} & & \\
& & \ddots & \\
0 & & & \Sigma_{k}^{-1}
\end{array}\right]
$$

where $\Sigma_{i}^{-1}=\frac{1}{\sigma^{2}}\left[I_{n_{i}}-\frac{\sigma_{a}^{2}}{\sigma^{2}+n_{i} \sigma_{a}^{2}} J_{n_{i}}\right]$. Using a well-known theorem in multivariate normal theory, the distribution of a given $\mathbf{y}$ is given by $N(\boldsymbol{\alpha}, A)$ where $\boldsymbol{\alpha}=\boldsymbol{\mu}_{a}+\Sigma_{12}^{\prime} \Sigma^{-1}(\mathbf{y}-\boldsymbol{\mu})$ and $A=\sigma_{a}^{2} I-\Sigma_{12}^{\prime} \Sigma^{-1} \Sigma_{12}$. It can be shown after some algebra that

$$
a_{i} \mid \mathbf{y} \stackrel{i . i . d}{\sim} N\left(w_{i} \mu+\left(1-w_{i}\right) \bar{y}_{i,}, v_{i}\right)
$$

where $w_{i}=\sigma^{2} /\left(\sigma^{2}+n_{i} \sigma_{a}^{2}\right), \bar{y}_{i .}=\left(\sum_{j=1}^{n_{i}} y_{i j}\right) / n_{i}$, and $v_{i}=w_{i} \sigma_{a}^{2}$. Recall that this conditional distribution was derived so that the expectations of $T_{1}, T_{2}$ and $T_{3}$ given $\mathbf{y}$ (or $\mathbf{y}_{\text {obs }}^{*}$ ) can be computed. These now follow easily. Thus the $\mathrm{t}^{\text {th }}$ iteration of the E-step is defined as

$$
\begin{aligned}
T_{1}^{(t)} & =\sum\left[w_{i}^{(t)} \mu^{(t)}+\left(1-w_{i}^{(t)}\right) \bar{y}_{i .}\right] \\
T_{2}^{(t)} & =\sum\left[w_{i}^{(t)} \mu^{(t)}+\left(1-w_{i}^{(t)}\right) \bar{y}_{i .}\right]^{2}+\sum v_{i}^{(t)} \\
T_{3}^{(t)} & =\sum_{i} \sum_{j}\left(y_{i j}-\bar{y}_{i .}\right)^{2}+\sum_{i} n_{i}\left[w_{i}^{(t)^{2}}\left(\mu^{(t)}-\bar{y}_{i .}\right)^{2}+v_{i}^{(t)}\right]
\end{aligned}
$$

Since the complete-data maximum likelihood estimates are

$$
\begin{aligned}
\hat{\mu} & =\frac{T_{1}}{k} \\
\hat{\sigma}_{a}^{2} & =\frac{T_{2}}{k}-\hat{\mu}^{2}
\end{aligned}
$$

and

$$
\hat{\sigma}^{2}=\frac{T_{3}}{N}
$$

the M-step is thus obtained by substituting the expectations for the sufficient statistics calculated in the E-step in the expressions for the maximum likelihood estimates:

$$
\begin{aligned}
\mu^{(t+1} & =\frac{T_{1}^{(t)}}{k} \\
\sigma_{a}^{2^{(t+1)}} & =\frac{T_{2}^{(t)}}{k}-\mu^{(t+1)^{2}} \\
\sigma^{2^{(t+1)}} & =\frac{T_{3}^{(t)}}{N}
\end{aligned}
$$

Iterations between these 2 sets of equations define the EM algorithm. With the starting values of $\mu^{(0)}=54.0, \sigma^{2^{(0)}}=70.0, \sigma_{a}^{2^{(0)}}=248.0$, the maximum likelihood estimates of $\hat{\mu}=53.3184, \hat{\sigma}_{a}^{2}=54.827$ and $\hat{\sigma}^{2}=249.22$ were obtained after 30 iterations. These can be compared with the estimates of $\sigma_{a}^{2}$ and $\sigma^{2}$ obtained by equating observed and expected mean squares from the random effects analysis of variance given above. Estimates of $\sigma_{a}^{2}$ and $\sigma^{2}$ obtained from this analysis are 73.39 and 248.29 respectively.

## Convergence of the EM Algorithm

The EM algorithm attempts to maximize $\ell_{\text {obs }}\left(\boldsymbol{\theta} ; \mathbf{y}_{\text {obs }}\right)$ by maximizing $\ell(\boldsymbol{\theta} ; \mathbf{y})$, the completedata log-likelihood. Each iteration of EM has two steps: an E-step and an M-step. The $t^{\text {th }}$ E-step finds the conditional expectation of the complete-data log-likelihood with respect to the conditional distribution of $\mathbf{y}$ given $\mathbf{y}_{\text {obs }}$ and the current estimated parameter $\boldsymbol{\theta}^{(t)}$ :

$$
\begin{aligned}
Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right) & =E_{\boldsymbol{\theta}^{(t)}}\left[\ell(\boldsymbol{\theta} ; \mathbf{y}) \mid \mathbf{y}_{\text {obs }}\right] \\
& =\int \ell(\boldsymbol{\theta} ; \mathbf{y}) f\left(\mathbf{y} \mid \mathbf{y}_{\text {obs }} ; \boldsymbol{\theta}^{(t)}\right) d \mathbf{y},
\end{aligned}
$$

as a function of $\boldsymbol{\theta}$ for fixed $\mathbf{y}_{\text {obs }}$ and fixed $\boldsymbol{\theta}^{(t)}$. The expectation is actually the conditional expectation of the complete-data log-likelihood, conditional on $\mathbf{y}_{\text {obs }}$.

The $t^{\text {th }} \mathrm{M}$-step then finds $\boldsymbol{\theta}^{(t+1)}$ to maximize $Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)$ i.e., finds $\boldsymbol{\theta}^{(t+1)}$ such that

$$
Q\left(\boldsymbol{\theta}^{(t+1)} ; \boldsymbol{\theta}^{(t)}\right) \geq Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)
$$

for all $\boldsymbol{\theta} \in \Theta$. To verify that this iteration produces a sequence of iterates that converges to a maximum of $\ell_{\text {obs }}\left(\boldsymbol{\theta} ; \mathbf{y}_{\text {obs }}\right)$, first note that by taking conditional expectation of both sides of

$$
\ell_{\text {obs }}\left(\boldsymbol{\theta} ; \mathbf{y}_{\text {obs }}\right)=\ell(\boldsymbol{\theta} ; \mathbf{y})-\log f_{2}\left(\mathbf{y}_{\text {mis }} \mid \mathbf{y}_{\text {obs }} ; \boldsymbol{\theta}\right),
$$

over the distribution of $\mathbf{y}$ given $\mathbf{y}_{\text {obs }}$ at the current estimate $\boldsymbol{\theta}^{(t)}, \ell_{\text {obs }}\left(\boldsymbol{\theta} ; \mathbf{y}_{\text {obs }}\right)$ can be expressed in the form

$$
\begin{aligned}
\ell_{\text {obs }}\left(\boldsymbol{\theta} ; \mathbf{y}_{\text {obs }}\right) & =\int \ell(\boldsymbol{\theta} ; \mathbf{y}) f\left(\mathbf{y} \mid \mathbf{y}_{\text {obs }} ; \boldsymbol{\theta}^{(t)}\right) d \mathbf{y}-\int \log f_{2}\left(\mathbf{y}_{\text {mis }} \mid \mathbf{y}_{\text {obs }} ; \boldsymbol{\theta}\right) f\left(\mathbf{y} \mid \mathbf{y}_{\text {obs }} ; \boldsymbol{\theta}^{(t)}\right) d \mathbf{y} \\
& =E_{\boldsymbol{\theta}^{(t)}}\left[\ell(\boldsymbol{\theta} ; \mathbf{y}) \mid \mathbf{y}_{\text {obs }}\right]-E_{\boldsymbol{\theta}^{(t)}}\left[\log f_{2}\left(\mathbf{y}_{\text {mis }} \mid \mathbf{y}_{\text {obs }} ; \boldsymbol{\theta}\right) \mid \mathbf{y}_{\text {obs }}\right] \\
& =Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)-H\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)
\end{aligned}
$$

where $Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)$ is as defined earlier and

$$
H\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)=E_{\boldsymbol{\theta}^{(t)}}\left[\log f_{2}\left(\mathbf{y}_{\text {mis }} \mid \mathbf{y}_{\text {obs }} ; \boldsymbol{\theta}\right) \mid \mathbf{y}_{\text {obs }}\right] .
$$

The following Lemma will be useful for proving a main result that the sequence of iterates $\boldsymbol{\theta}^{(t)}$ resulting from EM algrithm will converge at least to a local maximum of $\ell_{\text {obs }}\left(\boldsymbol{\theta} ; \mathbf{y}_{\text {obs }}\right)$.

Lemma: For any $\boldsymbol{\theta} \in \Theta$,

$$
H\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right) \leq H\left(\boldsymbol{\theta}^{(t)} ; \boldsymbol{\theta}^{(t)}\right)
$$

Theorem: The EM algorithm increases $\ell_{\text {obs }}\left(\boldsymbol{\theta} ; \mathbf{y}_{\text {obs }}\right)$ at each iteration, that is,

$$
\ell_{\text {obs }}\left(\boldsymbol{\theta}^{(t+1)} ; \mathbf{y}_{\text {obs }}\right) \geq \ell_{\text {obs }}\left(\boldsymbol{\theta}^{(t)} ; \mathbf{y}_{\text {obs }}\right)
$$

with equality if and only if

$$
Q\left(\boldsymbol{\theta}^{(t+1)} ; \boldsymbol{\theta}^{(t)}\right)=Q\left(\boldsymbol{\theta}^{(t)} ; \boldsymbol{\theta}^{(t)}\right)
$$

This Theorem implies that increasing $Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)$ at each step leads to maximizing or at least constantly increasing $\ell_{\text {obs }}\left(\boldsymbol{\theta} ; \mathbf{y}_{\text {obs }}\right)$.

Although the general theory of EM applies to any model, it is particularly useful when the complete data $\mathbf{y}$ are from an exponential family since, as seen in examples, in such cases the E-step reduces to finding the conditional expectation of the complete-data sufficient statistics, and the M-step is often simple. Nevertheless, even when the complete data $\mathbf{y}$ are from an exponential family, there exist a variety of important applications where complete-data maximum likelihood estimation itself is complicated; for example, see Little \& Rubin (1987) on selection models and log-linear models, which generally require iterative M-steps.

In a more general context, EM has been widely used in the recent past in computations related to Bayesian analysis to find the posterior mode of $\boldsymbol{\theta}$, which maximizes $\ell(\boldsymbol{\theta} \mid \mathbf{y})+\log p(\boldsymbol{\theta})$ for prior density $p(\boldsymbol{\theta})$ over all $\boldsymbol{\theta} \in \Theta$. Thus in Bayesian computations, log-likelihoods used above are substituted by log-posteriors.

## Convergence Rate of EM

EM algorithm implicitly defines a mapping

$$
\boldsymbol{\theta}^{(t+1)}=\boldsymbol{M}\left(\boldsymbol{\theta}^{(t)}\right) \quad t=0,1, \ldots
$$

where $\boldsymbol{M}(\boldsymbol{\theta})=\left(M_{1}(\boldsymbol{\theta}), \ldots, M_{d}(\boldsymbol{\theta})\right)$. For the problem of maximizing $Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)$, it can be shown that $\boldsymbol{M}$ has a fixed point and since $M$ is continuous and monotone $\boldsymbol{\theta}^{(t)}$ converges to a point $\boldsymbol{\theta}^{*} \in \Omega$. Consider the Taylor series expansion of

$$
\boldsymbol{\theta}^{(t+1)}=\boldsymbol{M}\left(\boldsymbol{\theta}^{(t)}\right)
$$

about $\boldsymbol{\theta}^{*}$, noting that $\boldsymbol{\theta}^{*}=M\left(\boldsymbol{\theta}^{*}\right)$ :

$$
\boldsymbol{M}\left(\boldsymbol{\theta}^{(t)}\right)=\boldsymbol{M}\left(\boldsymbol{\theta}^{*}\right)+\left.\left(\boldsymbol{\theta}^{(t)}-\boldsymbol{\theta}^{*}\right) \frac{\partial \boldsymbol{M}\left(\boldsymbol{\theta}^{(t)}\right)}{\partial \boldsymbol{\theta}}\right|_{\boldsymbol{\theta}=\boldsymbol{\theta}^{*}}
$$

which leads to

$$
\boldsymbol{\theta}^{(t+1)}-\boldsymbol{\theta}^{*}=\left(\boldsymbol{\theta}^{(t)}-\boldsymbol{\theta}^{*}\right) D M
$$

where $D M=\left.\frac{{ }_{\partial} \boldsymbol{M}\left(\boldsymbol{\theta}^{t}\right)}{\partial \boldsymbol{\theta}}\right|_{\boldsymbol{\theta}=\boldsymbol{\theta}^{*}}$ is a $d \times d$ matrix. Thus near $\boldsymbol{\theta}^{*}$, EM algorithm is essentially a linear iteration with the rate matrix $D M$.

Definition Recall that the rate of convergence of an iterative process is defined as

$$
\lim _{t \rightarrow \infty} \frac{\left\|\boldsymbol{\theta}^{(t+1)}-\boldsymbol{\theta}^{*}\right\|}{\left\|\boldsymbol{\theta}^{(t)}-\boldsymbol{\theta}^{*}\right\|}
$$

where $\|\cdot\|$ is any vector norm. For the EM algorithm, the rate of convergence is thus $r$

$$
r=\lambda_{\max }=\text { largest eigen value of } D M
$$

Dempster, Laird, and Rubin (1977) have shown that

$$
D M=\mathcal{I}_{m i s}\left(\boldsymbol{\theta}^{*} ; y_{o b s}\right) \mathcal{I}_{c}^{-1}\left(\boldsymbol{\theta}^{*} ; \boldsymbol{y}_{o b s}\right)
$$

Thus the rate of convergence is the largest eigen value of $\mathcal{I}_{\text {mis }}\left(\boldsymbol{\theta}^{*} ; \boldsymbol{y}_{\text {obs }}\right) \mathcal{I}_{c}^{-1}\left(\boldsymbol{\theta}^{*} ; \boldsymbol{y}_{\text {obs }}\right)$, where $\mathcal{I}_{\text {mis }}$ is the missing information matrix defined as

$$
\mathcal{I}_{m i s}\left(\boldsymbol{\theta} ; \boldsymbol{y}_{o b s}\right)=-E_{\boldsymbol{\theta}}\left\{\left.\frac{\partial^{2} f_{2}\left(\boldsymbol{y}_{m i s} \mid y_{o b s} ; \theta\right)}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^{T}} \right\rvert\, \boldsymbol{y}_{\text {obs }}\right\}
$$

and $\mathcal{I}_{c}$ is the conditional expected information matrix defined as

$$
\mathcal{I}_{c}\left(\boldsymbol{\theta} ; \boldsymbol{y}_{o b s}\right)=E_{\boldsymbol{\theta}}\left[I(\boldsymbol{\theta} ; \boldsymbol{y}) \mid \boldsymbol{y}_{o b s}\right]
$$

## EM Variants

## i. Generalized EM Algorithm (GEM)

Recall that in the M-step we maximize $Q\left(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}\right)$ i.e., find $\boldsymbol{\theta}^{(t+1)}$ s.t.

$$
Q\left(\boldsymbol{\theta}^{(t+1)} ; \boldsymbol{\theta}^{(t)}\right) \geq Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)
$$

for all $\boldsymbol{\theta}$. In the generalized version of the EM Algorithm we will require only that $\boldsymbol{\theta}^{(t+1)}$ be chosen such that

$$
Q\left(\boldsymbol{\theta}^{(t+1)} ; \boldsymbol{\theta}^{(t)}\right) \geq Q\left(\boldsymbol{\theta}^{(t)} ; \boldsymbol{\theta}^{(t)}\right)
$$

holds, i.e., $\boldsymbol{\theta}^{(t+1)}$ is chosen to increase $Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)$ over its value at $\boldsymbol{\theta}^{(t)}$ at each iteration $t$. This is sufficient to ensure that

$$
\ell\left(\boldsymbol{\theta}^{(t+1)} ; \boldsymbol{y}\right) \geq \ell\left(\boldsymbol{\theta}^{(t)} ; \boldsymbol{y}\right)
$$

at each iteration, so GEM sequence of iterates also converges to a local maximum.

## ii. GEM Algorithm based on a single N-R step

We use GEM-type algorithms when a global maximizer of $Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)$ does not exist in closed form. In this case, possibly an iterative method is required to accomplish the M-step, which might prove to be a computationally infeasible procedure. Since it is not essential to actually maximize $Q$ in a GEM, but only increase the likelihood, we may replace the M-step with a step that achieves that. One possibilty of such a step is a single iteration of the Newton-Raphson(N-R) algorithm, which we know is a descent method.

Let $\quad \boldsymbol{\theta}^{(t+1)}=\boldsymbol{\theta}^{(t)}+a^{(t)} \boldsymbol{\delta}^{(t)}$ where $\boldsymbol{\delta}^{(t)}=-\left[\frac{\partial^{2} Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^{T}}\right]_{\boldsymbol{\theta}=\boldsymbol{\theta}^{(t)}}^{-1}\left[\frac{\partial Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)}{\partial \boldsymbol{\theta}}\right] \quad \boldsymbol{\theta}=\boldsymbol{\theta}^{(t)}$
i.e., $\boldsymbol{\delta}^{(t)}$ is the N-R direction at $\boldsymbol{\theta}^{(t)}$ and $0<a^{(t)} \leq 1$. If $a^{(t)}=1$ this will define an exact N -R step. Here we will choose $a^{(t)}$ so that this defines a GEM sequence. This will be achieved if $a^{(t)}<2$ as $t \rightarrow \infty$.

## iii. Monte Carlo EM

The $t^{t h}$ iteration of the E-step can be modified by replacing $Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)$ with a Monte Carlo estimate obtained as follows:
(a) Draw samples of missing values $\mathbf{y}_{1}^{(t)}, \ldots, \mathbf{y}_{N}^{(t)}$ from $f_{2}\left(\mathbf{y}_{\text {mis }} \mid \mathbf{y}_{\text {obs }} ; \boldsymbol{\theta}\right)$. Each sample $\mathbf{y}_{j}^{(t)}$ is a vector of missing values needed to obtain a complete-data vector $\mathbf{y}_{j}=$ $\left(\mathbf{y}_{\text {obs }}, \mathbf{y}_{j}^{(t)}\right)$ for $j=1, \ldots, N$.
(b) Calculate

$$
\hat{Q}\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)=\frac{1}{N} \sum_{j=1}^{N} \log f\left(\mathbf{y}_{j} ; \boldsymbol{\theta}\right)
$$

where $\log f\left(\mathbf{y}_{j} ; \boldsymbol{\theta}\right)$ is the complete-data $\log$ likelihood evaluated at $\mathbf{y}_{j}$. It is recommended that $N$ be chosen to be small during the early EM iterations but increased as the EM iterations progress. Thus, MCEM estimate will move around initially and then converge as N increases later in the iterations.

## iv. ECM Algorithm

In this modification the M-step is replaced by a computationally simpler conditional maximization (CM) steps. Each CM step solves a simple optimization problem that may have an analytical solution or an elementary numerical solution(for e.g., a univariate optimization problem). The collection of the CM steps that follow the $t^{t h} \mathrm{E}$-step is called an $C M$ cycle. In each CM step, the conditional expectation of the complete-data log likelihood, $Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)$, computed in the preceding E-step is maximized subject to a constraint on $\Theta$. The union of all such constraints on $\Theta$ is such that the CM cycle results in the maximization over the entire parameter space $\Theta$.
Formally, let $S$ denote the total number of CM-steps in each cycle. Thus for $s=$ $1, \ldots, S$, the $s^{t h}$ CM-step in the $t^{t h}$ cycle requires the maximization of $Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)$ constrained by some function of $\boldsymbol{\theta}^{(t+(s-1) / S)}$, which is the maximiser from the $(s-1)^{t h}$ CM-step in the current cycle. That is, in the $s^{\text {th }}$ CM-step, find $\boldsymbol{\theta}^{(t+s / S)}$ in $\Theta$ such that

$$
Q\left(\boldsymbol{\theta}^{(t+s / S)} ; \boldsymbol{\theta}^{(t)}\right) \geq Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)
$$

for all $\boldsymbol{\theta} \in \Theta_{s}$. where $\Theta_{s}=\left\{\boldsymbol{\theta} \in \Theta: g_{s}(\boldsymbol{\theta})=g_{s}\left(\boldsymbol{\theta}^{(t+(s-1) / S)}\right)\right\}$. At the end of the $S$ cycles, $\boldsymbol{\theta}^{(t+1)}$ is set equal to the value obtained in the maximization in the last cycle $\boldsymbol{\theta}^{(t+(S / S)}$.

In order to understand this procedure, assume that $\boldsymbol{\theta}$ is partitioned into subvectors $\left(\boldsymbol{\theta}_{1}, \ldots, \boldsymbol{\theta}_{S}\right)$. Then at each step $s$ of the CM cycle, $Q\left(\boldsymbol{\theta} ; \boldsymbol{\theta}^{(t)}\right)$ is maximized with respect to $\boldsymbol{\theta}_{s}$ with the other components of $\boldsymbol{\theta}$ held fixed at their values from the previous CMsteps. Thus, in this case the constraint is induced by fixing $\left(\boldsymbol{\theta}_{1}, \ldots, \boldsymbol{\theta}_{s-1}, \boldsymbol{\theta}_{s+1}, \ldots, \boldsymbol{\theta}_{S}\right)$ at their current values.

## General Mixed Model

The general mixed linear model is given by

$$
\boldsymbol{y}=\boldsymbol{X} \boldsymbol{\beta}+\sum_{i=1}^{r} \boldsymbol{Z}_{i} \boldsymbol{u}_{i}+\boldsymbol{\epsilon}
$$

where $\boldsymbol{y}_{n \times 1}$ is an observed random vector, $\boldsymbol{X}$ is an $n \times p$, and $\boldsymbol{Z}_{i}$ are $n \times q_{i}$, matrices of known constants, $\boldsymbol{\beta}_{p \times 1}$ is a vector of unknown parameters, and $\boldsymbol{u}_{i}$ are $q_{i} \times 1$ are vectors of unobservable random effects.
$\boldsymbol{\epsilon}_{n \times 1}$ is assumed to be distributed $n$-dimensional multivariate normal $N\left(\mathbf{0}, \sigma_{0}^{2} \boldsymbol{I}_{n}\right)$ and each $\boldsymbol{u}_{i}$ are assumed to have $q_{i}$-dimensional multivariate normal distributions $N_{q_{i}}\left(\mathbf{0}, \sigma_{i}^{2} \boldsymbol{\Sigma}_{i}\right)$ for $i=1,2, \ldots, r$, independent of each other and of $\boldsymbol{\epsilon}$.

We take the complete data vector to be $\left(\boldsymbol{y}, \boldsymbol{u}_{1}, \ldots, \boldsymbol{u}_{r}\right)$ where $\boldsymbol{y}$ is the incomplete or the observed data vector. It can be shown easily that the covariance matrix of $\boldsymbol{y}$ is the $n \times n$ matrix $\boldsymbol{V}$ where

$$
\boldsymbol{V}=\sum_{i=1}^{r} \boldsymbol{Z}_{i} \boldsymbol{Z}_{i}^{T} \sigma_{i}^{2}+\sigma_{0}^{2} \boldsymbol{I}_{n}
$$

Let $q=\sum_{i=0}^{r} q_{i}$ where $q_{0}=n$. The joint distribution of $\boldsymbol{y}$ and $\boldsymbol{u}_{1}, \ldots, \boldsymbol{u}_{r}$ is $q$-dimensional multivariate normal $N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ where

$$
\underset{q \times 1}{\boldsymbol{\mu}}=\left[\begin{array}{c}
\boldsymbol{X} \boldsymbol{\beta} \\
\mathbf{0} \\
\vdots \\
\mathbf{0}
\end{array}\right] \quad \text { and } \quad \underset{\boldsymbol{\Sigma}}{ }{ }^{\boldsymbol{\Sigma}} \quad=\left[\begin{array}{cc}
\boldsymbol{V} & \left\{\sigma_{i}^{2} \boldsymbol{Z}_{i}\right\}_{i=1}^{r} \\
\left\{\sigma_{i}^{2} \boldsymbol{Z}_{i}^{T}\right\}_{i=1}^{r} & \left\{{ }_{d} \sigma_{i}^{2} \boldsymbol{I}_{q_{i}}\right\}_{i=1}^{r}
\end{array}\right]
$$

Thus the density function of $\boldsymbol{y}, \boldsymbol{u}, \ldots, \boldsymbol{u}_{r}$ is

$$
f\left(\boldsymbol{y}, \boldsymbol{u}_{1}, \boldsymbol{u}_{2}, \ldots, \boldsymbol{u}_{r}\right)=(2 \pi)^{-\frac{1}{2} q}|\boldsymbol{\Sigma}|^{-\frac{1}{2}} \exp \left(-\frac{1}{2} \boldsymbol{w}^{T} \boldsymbol{\Sigma}^{-1} \boldsymbol{w}\right)
$$

where $\boldsymbol{w}=\left[(\boldsymbol{y}-\boldsymbol{X} \boldsymbol{\beta})^{T}, u_{1}^{T}, \ldots, \boldsymbol{u}_{r}^{T}\right]$. This gives the complete data loglikelihood to be

$$
l=-\frac{1}{2} q \log (2 \pi)-\frac{1}{2} \sum_{i=0}^{r} q_{i} \log \sigma_{i}^{2}-\frac{1}{2} \sum_{i=0}^{r} \frac{\boldsymbol{u}_{i}^{T} \boldsymbol{u}_{i}}{\sigma_{i}^{2}}
$$

where $\boldsymbol{u}_{0}=\boldsymbol{y}-\boldsymbol{X} \boldsymbol{\beta}-\sum_{i=1}^{r} \boldsymbol{Z}_{i} \boldsymbol{u}_{i}=(\boldsymbol{\epsilon})$. Thus the sufficient statistics are: $\boldsymbol{u}_{i}^{T} \boldsymbol{u}_{i} i=0, \ldots, r$, and $\boldsymbol{y}-\sum_{i=1}^{r} \boldsymbol{Z}_{i} \boldsymbol{u}_{i}$ and the maximum likelihood estimates (m.l.e.'s) are

$$
\begin{aligned}
\hat{\sigma}_{i}^{2} & =\frac{\boldsymbol{u}_{i}^{T} \boldsymbol{u}_{i}}{q_{i}}, \quad i=0,1, \ldots, r \\
\hat{\boldsymbol{\beta}} & =\left(\boldsymbol{X}^{T} \boldsymbol{X}\right)^{-} \boldsymbol{X}^{T}\left(\boldsymbol{y}-\sum_{i=1}^{r} \boldsymbol{Z}_{i} \boldsymbol{u}_{i}\right)
\end{aligned}
$$

## Special Case: Two-Variance Components Model

The general mixed linear model reduces to:

$$
\boldsymbol{y}=\boldsymbol{X} \boldsymbol{\beta}+\boldsymbol{Z}_{1} \boldsymbol{u}_{1}+\boldsymbol{\epsilon} \quad \text { where } \quad \boldsymbol{\epsilon} \sim N\left(\mathbf{0}, \sigma_{0}^{2} \boldsymbol{I}\right) \quad \text { and } \quad \boldsymbol{u}_{1} \sim N\left(\mathbf{0}, \sigma_{1}^{2} \boldsymbol{I}_{n}\right)
$$

and the covariance matrix of $\boldsymbol{y}$ is now

$$
\boldsymbol{V}=\boldsymbol{Z}_{1} \boldsymbol{Z}_{1}^{T} \sigma_{1}^{2}+\sigma_{0}^{2} \boldsymbol{I}_{n}
$$

The complete data loglikelihood is

$$
l=-\frac{1}{2} q \log (2 \pi)-\frac{1}{2} \sum_{i=0}^{1} q_{i} \log \sigma_{i}^{2}-\frac{1}{2} \sum_{i=0}^{1} \frac{\boldsymbol{u}_{i}^{T} \boldsymbol{u}_{i}}{\sigma_{i}^{2}}
$$

where $\boldsymbol{u}_{0}=\boldsymbol{y}-\boldsymbol{X} \boldsymbol{\beta}-\boldsymbol{Z}_{1} \boldsymbol{u}_{1}$. The m.l.e.'s are

$$
\begin{aligned}
\hat{\sigma}_{i}^{2} & =\frac{\boldsymbol{u}_{i}^{T} \boldsymbol{u}_{i}}{q_{i}} \quad i=0,1 \\
\hat{\boldsymbol{\beta}} & =\left(\boldsymbol{X}^{T} \boldsymbol{X}\right)^{-} \boldsymbol{X}^{T}\left(\boldsymbol{y}-\boldsymbol{Z}_{1} \boldsymbol{u}_{1}\right)
\end{aligned}
$$

We need to find the expected values of the sufficient statistics $\boldsymbol{u}_{i}^{T} \boldsymbol{u}_{i}, \quad i=0,1$ and $\boldsymbol{y}-$ $Z_{1} \boldsymbol{u}_{1}$ conditional on observed data vector $\boldsymbol{y}$. Since $\boldsymbol{u}_{i} \mid \boldsymbol{y}$ is distributed as $q_{i}$-dimensional multivariate normal

$$
N\left(\sigma_{i}^{2} \boldsymbol{Z}_{i}^{T} \boldsymbol{V}^{-1}(\boldsymbol{y}-\boldsymbol{X} \boldsymbol{\beta}), \sigma_{i}^{2} \boldsymbol{I}_{q_{i}}-\sigma_{i}^{4} \boldsymbol{Z}_{i}^{T} \boldsymbol{V}^{-1} \boldsymbol{Z}_{i}\right)
$$

we have

$$
\begin{aligned}
E\left(\boldsymbol{u}_{i}^{T} \boldsymbol{u}_{i} \mid \boldsymbol{y}\right) & =\sigma_{i}^{4}(\boldsymbol{y}-\boldsymbol{X} \boldsymbol{\beta})^{T} \boldsymbol{V}^{-1} \boldsymbol{Z}_{i} \boldsymbol{Z}_{i}^{T} \boldsymbol{V}^{-1}(\boldsymbol{y}-\boldsymbol{X} \boldsymbol{\beta})+\operatorname{tr}\left(\sigma_{i}^{2} \boldsymbol{I}_{q_{i}}-\sigma_{i}^{4} \boldsymbol{Z}_{i}^{T} \boldsymbol{V}^{-1} \boldsymbol{Z}_{i}\right) \\
E\left(\boldsymbol{y}-\boldsymbol{Z}_{1} \boldsymbol{u}_{1} \mid \boldsymbol{y}\right) & =\boldsymbol{X} \boldsymbol{\beta}+\sigma_{0}^{2} \boldsymbol{V}^{-1}(\boldsymbol{y}-\boldsymbol{X} \boldsymbol{\beta})
\end{aligned}
$$

noting that

$$
\begin{aligned}
& E\left(\boldsymbol{u}_{0} \mid \boldsymbol{y}\right)=\sigma_{0}^{2} \boldsymbol{V}^{-1}(\boldsymbol{y}-\boldsymbol{X} \boldsymbol{\beta})
\end{aligned}
$$

where $\boldsymbol{Z}_{0}=\boldsymbol{I}_{n}$.

From the above we can derive the following EM-type algorithms for this case:

## Basic EM Algorithm

Step 1 (E-step) Set $\boldsymbol{V}^{(t)}=\boldsymbol{Z}_{1} \boldsymbol{Z}_{1}^{\prime} \sigma_{1}^{2^{(t)}}+\sigma_{0}^{2(t)} \boldsymbol{I}_{n}$ and for $i=0,1$ calculate

$$
\begin{aligned}
\hat{s}_{i}^{(t)}= & \left.E\left(\boldsymbol{u}_{i}^{T} \boldsymbol{u}_{i} \mid \boldsymbol{y}\right)\right|_{\boldsymbol{\beta}=\boldsymbol{\beta}^{(t)}, \sigma_{i}^{2}=\sigma_{i}^{2(t)}} \\
= & \sigma_{i}^{4^{(t)}}\left(\boldsymbol{y}-\boldsymbol{X} \boldsymbol{\beta}^{(t)}\right)^{T} \boldsymbol{V}^{(t)} \boldsymbol{Z}_{i} \boldsymbol{Z}_{i}^{T} \boldsymbol{V}^{(t)}\left(\boldsymbol{y}-\boldsymbol{X} \boldsymbol{\beta}^{(t)}\right) \\
& +\operatorname{tr}\left(\sigma_{i}^{2^{2(t)}} \boldsymbol{I}_{q_{i}}-\sigma_{i}^{4^{(t)}} \boldsymbol{Z}_{i}^{T} \boldsymbol{V}^{(t)^{-1}} \boldsymbol{Z}_{i}\right) i=0,1 \\
\hat{\boldsymbol{w}}^{(t)}= & \left.E\left(\boldsymbol{y}-\boldsymbol{Z}_{1} \boldsymbol{u}_{1} \mid \boldsymbol{y}\right)\right|_{\boldsymbol{\beta}=\boldsymbol{\beta}^{(t)}, \sigma_{i}^{2}=\sigma_{i}^{2(t)}} \\
= & \boldsymbol{X} \boldsymbol{\beta}^{(t)}+\sigma_{0}^{2^{(t)}} \boldsymbol{V}^{(t)^{-1}}\left(\boldsymbol{y}-\boldsymbol{X} \boldsymbol{\beta}^{(t)}\right)
\end{aligned}
$$

Step 2 (M-step)

$$
\begin{aligned}
\sigma_{i}^{2^{(t+1)}} & =\hat{s}_{i}^{(t)} / q_{i} \quad i=0,1 \\
\boldsymbol{\beta}^{(t+1)} & =\left(\boldsymbol{X}^{T} \boldsymbol{X}\right)^{-1} \boldsymbol{X}^{\prime} \hat{\boldsymbol{w}}^{(t)}
\end{aligned}
$$

## ECM Algorithm

Step 1 (E-step) Set $\boldsymbol{V}^{(t)}=\boldsymbol{Z}_{1} \boldsymbol{Z}_{1}^{\prime} \sigma_{1}^{2^{(t)}}+\sigma_{0}^{2^{(t)}} \boldsymbol{I}_{n}$ and, for $i=0$, 1 calculate

$$
\begin{aligned}
\hat{s}_{i}^{(t)}= & \left.E\left(\boldsymbol{u}_{i}^{T} \boldsymbol{u}_{i} \mid \boldsymbol{y}\right)\right|_{\boldsymbol{\beta}=\boldsymbol{\beta}^{(t)}, \sigma_{i}^{2}=\sigma_{i}^{2(t)}} \\
= & \sigma_{i}^{4^{(t)}}\left(y-\boldsymbol{X} \boldsymbol{\beta}^{(t)}\right)^{T} \boldsymbol{V}^{(t)^{-1}} \boldsymbol{Z}_{i} \boldsymbol{Z}_{i} \boldsymbol{V}^{(t))^{-1}}(\boldsymbol{y}-\boldsymbol{X} \boldsymbol{\beta}) \\
& +\operatorname{tr}\left(\sigma_{i}^{2^{(t)}} \boldsymbol{I}_{q_{i}}-\sigma_{i}^{4^{(t)}} \boldsymbol{Z}_{i}^{T} \boldsymbol{V}^{(t)^{-1}} \boldsymbol{Z}_{i}\right)
\end{aligned}
$$

## Step 2 (M-step)

Partition the parameter vector $\boldsymbol{\theta}=\left(\sigma_{0}^{2}, \sigma_{1}^{2}, \boldsymbol{\beta}\right)$ as $\boldsymbol{\theta}_{1}=\left(\sigma_{0}^{2}, \sigma_{1}^{2}\right)$ and $\boldsymbol{\theta}_{2}=\boldsymbol{\beta}$

## CM-step 1

Maximize complete data log likelihood over $\boldsymbol{\theta}_{1}$

$$
\sigma_{i}^{2^{(t+1)}}=\hat{s}_{i}^{(t)} / q_{i} \quad i=0,1
$$

## CM-step 2

Calculate $\boldsymbol{\beta}^{(t+1)}$ as

$$
\boldsymbol{\beta}^{(t+1)}=\left(\boldsymbol{X}^{T} \boldsymbol{X}\right)^{-1} \boldsymbol{X}^{T} \hat{\boldsymbol{w}}^{(t+1)}
$$

where

$$
\hat{\boldsymbol{w}}^{(t+1)}=\boldsymbol{X} \boldsymbol{\beta}^{(t)}+\sigma_{0}^{2(t+1)} \boldsymbol{V}^{(t+1)^{-1}}\left(\boldsymbol{y}-\boldsymbol{X} \boldsymbol{\beta}^{(t)}\right)
$$

## ECME Algorithm

Step 1 (E-step) Set $\boldsymbol{V}^{(t)}=\boldsymbol{Z}_{1} \boldsymbol{Z}_{1}^{\prime} \sigma_{1}^{2^{(t)}}+\sigma_{0}^{2^{(t)}} \boldsymbol{I}_{n}$ and, for $i=0$, 1 calculate

$$
\begin{aligned}
\hat{s}_{i}^{(t)} & =E\left(\boldsymbol{u}_{i}^{T} \boldsymbol{u}_{i} \mid \boldsymbol{y}\right) \mid \sigma_{i}^{2}=\sigma_{i}^{2(t)} \\
& =\sigma_{i}^{4^{(t)}} \boldsymbol{y}^{T} \boldsymbol{P}^{(t)} \boldsymbol{Z}_{i} \boldsymbol{Z}_{i}^{T} \boldsymbol{P}^{(t)} \boldsymbol{y}+\operatorname{tr}\left(\sigma_{i}^{2^{(t)}} \boldsymbol{I}_{q_{i}}-\sigma_{i}^{4^{(t)}} \boldsymbol{Z}_{i}^{T} \boldsymbol{V}^{(t)^{-1}} \boldsymbol{Z}_{i}\right)
\end{aligned}
$$

where $\boldsymbol{P}^{(t)}=\boldsymbol{V}^{(t)^{-1}}-\boldsymbol{V}^{(t)^{-1}} \boldsymbol{X}\left(\boldsymbol{X}^{T} \boldsymbol{V}^{(t)^{-1}} \boldsymbol{X}\right)^{-} \boldsymbol{X}^{T} \boldsymbol{V}^{(t)^{-1}}$

## Step 2 (M-step)

Partition $\boldsymbol{\theta}$ as $\boldsymbol{\theta}_{1}=\left(\sigma_{0}^{2}, \sigma_{1}^{2}\right)$ and $\boldsymbol{\theta}_{2}=\boldsymbol{\beta}$ as in ECM.

## CM-step 1

Maximize complete data $\log$ likelihood over $\boldsymbol{\theta}_{1}$

$$
\sigma_{i}^{2^{(t+1)}}=\hat{s}_{i}^{(t)} / q_{i} \quad i=0,1
$$

## CM-step 2

Maximize the observed data log likelihood over $\boldsymbol{\theta}$ given $\boldsymbol{\theta}_{1}^{(t)}=\left(\sigma_{0}^{2^{(t)}}, \sigma_{0}^{\left.2^{(t)}\right)}\right.$ :

$$
\boldsymbol{\beta}^{(t+1)}=\left(\boldsymbol{X}^{T} \boldsymbol{V}^{(t+1)^{-1}} \boldsymbol{X}\right)^{-1}\left(\boldsymbol{X}^{T} \boldsymbol{V}^{(t+1)^{-1}}\right) \boldsymbol{y}
$$

(Note: This is the WLS estimator of $\boldsymbol{\beta}$.)

## Example of Mixed Model Analysis using the EM Algorithm

The first example is an evaluation of the breeding value of a set of five sires in raising pigs, taken from Snedecor and Cochran (1967). (The data is reported in Appendix 4.) The experiment was designed so that each sire is mated to a random group of dams, each mating producing a litter of pigs whose characteristics are criterion. The model to be estimated is

$$
\begin{equation*}
y_{i j k}=\mu+\alpha_{i}+\beta_{i j}+\epsilon_{i j k}, \tag{4}
\end{equation*}
$$

where $\alpha_{i}$ is a constant associated with the $i$-th sire effect, $\beta_{i j}$ is a random effect associated with the $i$-th sire and $j$-th dam, $\epsilon_{i j k}$ is a random term. The three different initial values for $\left(\sigma_{0}^{2}, \sigma_{1}^{2}\right)$ are $(1,1),(10,10)$ and $(.038, .0375)$; the last initial value corresponds to the estimates from the SAS ANOVA procedure.

## Table 1: Average Daily Gain of Two Pigs of Each Litter (in pounds)

| Sire | Dam | Gain |
| :---: | :---: | :---: |
| 1 | 1 | 2.77 |
| 1 | 1 | 2.38 |
| 1 | 2 | 2.58 |
| 1 | 2 | 2.94 |
| 2 | 1 | 2.28 |
| 2 | 1 | 2.22 |
| 2 | 2 | 3.01 |
| 2 | 2 | 2.61 |
| 3 | 1 | 2.36 |
| 3 | 1 | 2.71 |


| Sire | Dam | Gain |
| :---: | :---: | :---: |
| 3 | 2 | 2.72 |
| 3 | 2 | 2.74 |
| 4 | 1 | 2.87 |
| 4 | 1 | 2.46 |
| 4 | 2 | 2.31 |
| 4 | 2 | 2.24 |
| 5 | 1 | 2.74 |
| 5 | 1 | 2.56 |
| 5 | 2 | 2.50 |
| 5 | 2 | 2.48 |

```
###########################################################
# Classical EM algorithm for Linear Mixed Model #
###########################################################
em.mixed <- function(y, x, z, beta, var0, var1,maxiter=2000,tolerance = 1e-0010)
    {
    time <-proc.time()
    n <- nrow(y)
    q1 <- nrow(z)
    conv <- 1
    LO <- loglike(y, x, z, beta, var0, var1)
    i<-0
    cat(" Iter. sigma0 sigma1 Likelihood",fill=T)
    repeat {
        if(i>maxiter) {conv<-0
                break}
    V <- c(var1) * z %*% t(z) + c(var0) * diag(n)
    Vinv <- solve(V)
    xb <- x %*% beta
    resid <- (y-xb)
    temp1 <- Vinv %*% resid
    s0 <- c(var0)^2 * t(temp1)%*%temp1 + c(var0) * n - c(var0)^2 * tr(Vinv)
    s1 <- c(var1)^2 * t(temp1)%*%z%**%t(z)%*%temp1+ c(var1)*q1 -
                                    c(var1)^2 *tr(t(z)%*%Vinv%*%z)
    w <- xb + c(var0) * temp1
    var0 <- s0/n
    var1 <- s1/q1
    beta <- ginverse( t(x) %*% x) %*% t(x)%*% w
    L1 <- loglike(y, x, z, beta, var0, var1)
    if(L1 < L0) { print("log-likelihood must increase, llikel <llikeO, break.")
                        conv <- 0
                        break
                        }
    i <- i + 1
    cat(" ", i," ",var0," ",var1," ",L1,fill=T)
    if(abs(L1 - L0) < tolerance) {break} #check for convergence
    L0 <- L1
    }
list(beta=beta, var0=var0,var1=var1,Loglikelihood=LO)
}
```

```
#########################################################
# loglike calculates the LogLikelihood for Mixed Model #
#############################################################
loglike<- function(y, x, z, beta, var0, var1)
    {
    n<- nrow(y)
    V <- c(var1) * z %*% t(z) + c(var0) * diag(n)
    Vinv <- ginverse(V)
    xb <- x %*% beta
    resid <- (y-xb)
    temp1 <- Vinv %*% resid
    (-.5)*( log(det(V)) + t(resid) %*% temp1 )
}
> y <- matrix(c(2.77, 2.38, 2.58, 2.94, 2.28, 2.22, 3.01, 2.61,
+ 2.36, 2.71, 2.72, 2.74, 2.87, 2.46, 2.31, 2.24,
+ 2.74, 2.56, 2.50, 2.48),20,1)
> x1 <- rep(c(1,0,0,0,0),rep(4,5))
> x2 <- rep(c(0,1,0,0,0),rep(4,5))
> x3 <- rep(c(0,0,1,0,0),rep(4,5))
> x4 <- rep(c(0,0,0,1,0),rep(4,5))
> x <- cbind(1,x1,x2,x3,x4)
>x
    x1 x2 x3 x4
[1,] 1 1 0 0 0
[2,] 1 1 0 0 0
[3,] 1 1 0 0 0
[4,] 1 1 0 0 0
[5,] 1 0 1 0 0
[6,] 1 0
[7,] 1 00 1 0
[8,] 1 0 1 0 0
[9,] 1 0 0 0 1 0
[10,] 1 0 0 1 0
[11,] 1 0 0 1 0
[12,] 1 0 0 1 0
[13,] 1 0 0 0 1
[14,] 1 0 0 0 1
```

```
[15,] 1 0 0 0 1
[16,] 1 0 0 0 1
[17,] 1 0 0 0 0
[18,] 1 0 0 0 0
[19,] 1 0 0 0 0
[20,] 1 0 0 0 0
```

```
> beta <- lm(y~ x1 + x2 + x3 +x4)$coefficients
> beta
    [,1]
(Intercept) 2.5700
    x1 0.0975
    x2 -0.0400
    x3 0.0625
    x4 -0.1000
```

> $z=$ matrix $(r e p(\operatorname{as.vector}(\operatorname{diag}(1,10)), r e p(2,100)), 20,10)$
$>\mathrm{z}$

|  | $[, 1]$ | $[, 2]$ | $[, 3]$ | $[, 4]$ | $[, 5]$ | $[, 6]$ | $[, 7]$ | $[, 8]$ | $[, 9]$ | $[, 10]$ |
| :---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| $[1]$, | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $[2]$, | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $[3]$, | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $[4]$, | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $[5]$, | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $[6]$, | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| $[7]$, | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| $[8]$, | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| $[9]$, | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 |
| $[10]$, | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 |
| $[11]$, | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 |
| $[12]$, | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 0 |
| $[13]$, | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 |
| $[14]$, | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 |
| $[15]$, | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 |
| $[16]$, | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 |
| $[17]$, | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 |
| $[18]$, | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 |
| $[19]$, | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 |
| $[20]$, | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 |

```
> tolerance <- 1e-0010
> maxiter <- 2000
> seed <- 100
```

```
> tr <- function(x) sum(diag(x))
```

> pig.em.results=em.mixed ( $\mathrm{y}, \mathrm{x}, \mathrm{z}$, beta, 1,1 )

| Iter. | sigma0 | sigma1 | Likelihood |
| :---: | :---: | :---: | :---: |
| 1 | 0.355814166666667 | 0.672928333333333 | 1.79926992591149 |
| 2 | 0.161289219777595 | 0.415630697486737 | 7.67656899233908 |
| 3 | 0.0876339412658286 | 0.251467232868861 | 12.1211098467902 |
| 4 | 0.0572854577134676 | 0.154608860144254 | 15.1706421424132 |
| 5 | 0.0442041832136993 | 0.0994160507019009 | 17.130593350043 |
| 6 | 0.0383642480366208 | 0.0681788894372488 | 18.3694784469532 |
| 7 | 0.0356787493219611 | 0.0501555498139391 | 19.1464492643216 |
| 8 | 0.0344485615271845 | 0.0393230630005528 | 19.630522654304 |
| 9 | 0.0339421060204835 | 0.032463488015722 | 19.9344237098546 |
| 10 | 0.0338157550885801 | 0.0278799360094821 | 20.1296516102853 |
| 11 | 0.0338906702246361 | 0.0246617461868549 | 20.2590878975877 |
| 12 | 0.0340677808426562 | 0.0223026501468333 | 20.3478401280992 |
| 13 | 0.0342914060268899 | 0.02050908367209 | 20.4106731999847 |
| 14 | 0.0345307406853334 | 0.0191033399491361 | 20.4564548122603 |
| 15 | 0.0347693177408093 | 0.0179733335898586 | 20.4906651701558 |
| 16 | 0.0349988121264555 | 0.0170456362588657 | 20.5167959381214 |
| 17 | 0.0352154250729573 | 0.0162704665032569 | 20.5371387472463 |
| 18 | 0.0354178131324059 | 0.0156130259538466 | 20.5532397057213 |
| 19 | 0.035605923319033 | 0.0150483214110959 | 20.5661685104734 |
| 20 | 0.0357803477632565 | 0.0145579670979211 | 20.5766822585211 |
| . |  |  |  |
| . |  |  |  |
|  |  |  |  |
| 56 | 0.0381179518848995 | 0.00973330752818472 | $2 \quad 20.6382666130708$ |
| 57 | 0.0381395936235214 | 0.00969817892685448 | 820.6383975558995 |
| 58 | 0.0381603337241741 | 0.00966462573503992 | 220.6385178920802 |
| 59 | 0.0381802168890155 | 0.00963256091234115 | $5 \quad 20.6386285603282$ |
| 60 | 0.0381992850741614 | 0.00960190350873251 | 120.6387304072052 |
| 61 | 0.0382175776978136 | 0.00957257813571635 | 520.6388241972305 |
| 62 | 0.0382351318295782 | 0.00954451449226923 | $3 \quad 20.6389106217546$ |
| 63 | 0.0382519823629303 | 0.0095176469390277 | 20.6389903067599 |
| 64 | 0.0382681621725531 | 0.00949191411504429 | 920.639063819736 |
| 65 | 0.0382837022580806 | 0.00946725859219654 | 420.639131675748 |
| 66 | 0.0382986318756009 | 0.00944362656297278 | $8 \quad 20.6391943428055$ |
| 67 | 0.038312978658123 | 0.00942096755790665 | 20.6392522466191 |
| 68 | 0.0383267687260784 | 0.00939923418940295 | 520.6393057748245 |
| 69 | 0.0383400267888113 | 0.0093783819191014 | 20.6393552807376 |
| 70 | 0.0383527762379075 | 0.00935836884627387 | $7 \quad 20.6394010866997$ |
| 71 | 0.0383650392331249 | 0.00933915551505174 | 420.6394434870619 |
| 72 | 0.0383768367816026 | 0.00932070473854103 | 320.639482750852 |
| 73 | 0.0383881888109615 | 0.00930298143810976 | $6 \quad 20.6395191241599$ |
| 74 | 0.0383991142368419 | 0.00928595249632906 | 620.6395528322763 |
| 75 | 0.0384096310253713 | 0.00926958662222157 | $7 \quad 20.6395840816114$ |
| 76 | 0.0384197562510039 | 0.00925385422762105 | 520.6396130614187 |


| 77 | 0.0384295061501315 | 0.00923872731357883 | 20.6396399453462 |
| :---: | :---: | :---: | :---: |
| 78 | 0.0384388961708265 | 0.00922417936586811 | 20.6396648928339 |
| 79 | 0.0384479410190403 | 0.00921018525873869 | 20.6396880503735 |
| 80 | 0.038456654701554 | 0.00919672116616442 | 20.639709552647 |
| 81 | 0.0384650505659457 | 0.00918376447990421 | 20.6397295235547 |
| - |  |  |  |
| - |  |  |  |
| . |  |  |  |
| 148 | 0.0386757695291326 | 0.00886369156913502 | 20.6399971471733 |
| 149 | 0.038676564371102 | 0.00886250240210069 | 20.6399973283659 |
| 150 | 0.0386773329964768 | 0.00886135258462483 | 20.6399974978113 |
| 151 | 0.0386780762792084 | 0.00886024079675071 | 20.6399976562748 |
| 152 | 0.0386787950635179 | 0.00885916576395544 | 20.6399978044714 |
| 153 | 0.0386794901649452 | 0.00885812625551144 | 20.6399979430694 |
| 154 | 0.0386801623713602 | 0.00885712108291183 | 20.6399980726932 |
| 155 | 0.0386808124439345 | 0.00885614909835692 | 20.6399981939264 |
| 156 | 0.0386814411180777 | 0.00885520919329904 | 20.6399983073142 |
| 157 | 0.0386820491043391 | 0.0088543002970433 | 20.6399984133665 |
| 158 | 0.0386826370892749 | 0.00885342137540194 | 20.6399985125595 |
| 159 | 0.0386832057362845 | 0.00885257142939978 | 20.6399986053387 |
| 160 | 0.0386837556864153 | 0.0088517494940289 | 20.6399986921201 |
| 161 | 0.0386842875591385 | 0.00885095463705022 | 20.639998773293 |
| 162 | 0.038684801953096 | 0.00885018595784018 | 20.6399988492209 |
| 163 | 0.0386852994468205 | 0.0088494425862806 | 20.6399989202439 |
| 164 | 0.0386857805994294 | 0.00884872368168998 | 20.6399989866798 |
| 165 | 0.0386862459512932 | 0.00884802843179444 | 20.6399990488258 |
| 166 | 0.0386866960246808 | 0.00884735605173682 | 20.6399991069597 |
| 167 | 0.03868713132438 | 0.0088467057831223 | 20.6399991613413 |
| 168 | 0.0386875523382973 | 0.00884607689309907 | 20.6399992122135 |
| 169 | 0.0386879595380351 | 0.00884546867347273 | 20.6399992598033 |
| 170 | 0.0386883533794493 | 0.00884488043985296 | 20.639999304323 |
| 171 | 0.0386887343031859 | 0.00884431153083127 | 20.6399993459712 |
| - |  |  |  |
| - | . |  |  |
|  |  |  |  |
| 200 | 0.0386957009460699 | 0.00883391223498804 | 20.6399998631143 |
| 201 | 0.0386958413121088 | 0.00883370281147353 | 20.6399998687721 |
| 202 | 0.0386959770906578 | 0.00883350023633904 | 20.6399998740661 |
| 203 | 0.0386961084319343 | 0.00883330428508165 | 20.6399998790199 |
| 204 | 0.0386962354812184 | 0.00883311474059363 | 20.6399998836552 |
| 205 | 0.0386963583790162 | 0.00883293139291657 | 20.6399998879925 |
| 206 | 0.0386964772612182 | 0.00883275403900379 | 20.6399998920511 |
| 207 | 0.0386965922592513 | 0.00883258248249084 | 20.6399998958488 |
| 208 | 0.038696703500227 | 0.0088324165334737 | 20.6399998994025 |
| 209 | 0.0386968111070837 | 0.00883225600829448 | 20.6399999027278 |
| 210 | 0.0386969151987245 | 0.00883210072933436 | 20.6399999058394 |
| 211 | 0.0386970158901508 | 0.00883195052481344 | 20.639999908751 |
| 212 | 0.0386971132925907 | 0.00883180522859742 | 20.6399999114756 |
| 213 | 0.0386972075136236 | 0.00883166468001066 | 20.6399999140251 |
| 214 | 0.0386972986573006 | 0.0088315287236556 | 20.6399999164108 |
| 215 | 0.0386973868242609 | 0.00883139720923821 | 20.6399999186432 |
| 216 | 0.0386974721118441 | 0.00883126999139926 | 20.6399999207322 |
| 217 | 0.0386975546141991 | 0.00883114692955128 | 20.639999922687 |
| 218 | 0.0386976344223887 | 0.00883102788772094 | 20.6399999245163 |


| 219 | 0.0386977116244922 | 0.00883091273439672 | 20.639999926228 |
| :---: | :---: | :---: | :---: |
| . |  |  |  |
| - |  |  |  |
|  |  |  |  |
| 243 | 0.0386989678273622 | 0.00882903917935159 | 20.6399999460984 |
| 244 | 0.0386990015024108 | 0.00882898895948373 | 20.6399999464241 |
| 245 | 0.0386990340785396 | 0.00882894037866968 | 20.6399999467289 |
| 246 | 0.0386990655916262 | 0.00882889338338294 | 20.6399999470141 |
| 247 | 0.038699096076376 | 0.00882884792184704 | 20.639999947281 |
| 248 | 0.0386991255663601 | 0.00882880394397821 | 20.6399999475308 |
| 249 | 0.038699154094053 | 0.00882876140132994 | 20.6399999477646 |
| 250 | 0.0386991816908679 | 0.00882872024703932 | 20.6399999479833 |
| 251 | 0.0386992083871918 | 0.00882868043577519 | 20.639999948188 |
| 252 | 0.0386992342124192 | 0.00882864192368795 | 20.6399999483796 |
| 253 | 0.0386992591949842 | 0.00882860466836104 | 20.6399999485588 |
| 254 | 0.0386992833623921 | 0.00882856862876405 | 20.6399999487266 |
| 255 | 0.0386993067412498 | 0.00882853376520732 | 20.6399999488836 |
| 256 | 0.0386993293572951 | 0.00882850003929805 | 20.6399999490305 |
| 257 | 0.0386993512354253 | 0.00882846741389785 | 20.639999949168 |
| 258 | 0.0386993723997246 | 0.00882843585308171 | 20.6399999492966 |
| 259 | 0.0386993928734904 | 0.00882840532209825 | 20.639999949417 |
| 260 | 0.0386994126792596 | 0.00882837578733138 | 20.6399999495297 |
| 261 | 0.0386994318388329 | 0.00882834721626309 | 20.6399999496351 |
| 262 | 0.0386994503732993 | 0.00882831957743758 | 20.6399999497338 |

> pig.em.results

## \$beta:

$$
[, 1]
$$

[1,] 2.5700
[2,] 0.0975
[3,] -0.0400
[4,] 0.0625
[5,] -0.1000
$\$ \operatorname{var} 0$ :

## [,1]

[1,] 0.03869945

## \$var1:

[,1]
[1,] 0.00882832
\$Loglikelihood:
[,1]
[1,] 20.64

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