The Method of Scoring. The EM Algorithm

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The method of scoring

The iteration

$$\theta \leftarrow \theta + j_n(\theta)^{-1} S(\theta)$$

has a tendency to be unstable for many reasons, one of them being that $j_n(\theta)$ may be negative unless θ already is very close to to the MLE $\hat{\theta}$. In addition, $j(\theta)$ might sometimes be hard to calculate.

R. A. Fisher introduced the *method of scoring* which simply replaces the observed second derivative with its expectation to yield the iteration

$$\theta \leftarrow \theta + i_n(\theta)^{-1} S(\theta)$$

which in the case of independent and identically distributed

observations gives

$$\theta \leftarrow \theta + i(\theta)^{-1} S(\theta) / n$$
.

In many cases, $i(\theta)$ is easier to calculate and $i(\theta)$ is always positive.

In canonical exponential families we get

$$j(\theta) = \frac{\partial^2}{\partial \theta^2} \{ c(\theta) - \theta t(X) \} = c''(\theta) = i(\theta)$$

so for canonical exponential families the method of scoring and the method of Newton–Raphson coincide.

If we let $v(\theta) = c''(\theta)$ the iteration becomes

$$\theta \leftarrow \theta + v(\theta)^{-1} S(\theta) / n.$$

The identity of Newton–Raphson and the method of scoring only holds for the canonical parameter. If $\theta=g(\mu)$

$$\begin{split} j(\mu) &= \frac{\partial^2}{\partial \mu^2} \{ c(g(\mu)) - g(\mu) t(X) \} \\ &= \frac{\partial}{\partial \mu} \left[g'(\mu) \tau \{ g(\mu) \} - g'(\mu) t(X) \right] \\ &= v \{ g(\mu) \} \{ g'(\mu) \}^2 + g''(\mu) \left[\tau \{ g(\mu) \} - t(X) \right]. \end{split}$$

The method of scoring is simpler because the last term has expectation equal to 0:

$$i(\mu) = \mathbf{E}\{j(\mu)\} = v\{q(\mu)\}\{q'(\mu)\}^2.$$

The method of scoring is used in the glim procedure for estimation in so-called *generalised linear models*.

The EM algorithm

The EM algorithm is a supplement or alternative to Newton–Raphson in cases where the complications in calculating the MLE are due to *incomplete observation*.

Data (X,Y) are the *complete data* whereas only incomplete data Y=y are observed.

The complete data log-likelihood is:

$$l(\theta) = \log L(\theta; x, y) = \log f(x, y; \theta).$$

The marginal log-likelihood or incomplete data log-likelihood is based on y alone and is equal to

$$l_y(\theta) = \log L(\theta; y) = \log f(y; \theta).$$

We wish to maximize l_y in θ but l_y is typically quite unpleasant:

$$l_y(\theta) = \log \int f(x, y; \theta) dx.$$

The EM algorithm is a method of maximizing the latter iteratively and alternates between two steps, one known as the E-step and one as the M-step, to be detailed below.

We let θ^* be and arbitrary but fixed value, typically the value of θ at the current iteration.

The E-step calculates the expected complete data log-likelihood ratio $q(\theta \mid \theta^*)$:

$$q(\theta \mid \theta^*) = \mathbf{E}_{\theta^*} \left[\log \frac{f(X, y; \theta)}{f(X, y; \theta^*)} \mid Y = y \right]$$
$$= \int \log \frac{f(x, y; \theta)}{f(x, y; \theta^*)} f(x \mid y; \theta^*) dx.$$

The M-step maximizes $q(\theta \,|\, \theta^*)$ in θ for for fixed θ^* , i.e. calculates

$$\theta^{**} = \arg \max_{\theta} q(\theta \mid \theta^*).$$

We will show that after an E-step and subsequent M-step, the likelihood function has never decreased.

Kullback-Leibler divergence

The KL divergence between f and g is

$$KL(f:g) = \int f(x) \log \frac{f(x)}{g(x)} dx.$$

Also known as $relative\ entropy\ of\ g$ with respect to f.

Since $-\log x$ is a convex function, Jensen's inequality gives

 $KL(f:g) \ge 0$ and KL(f:g) = 0 if and only if f = g, since

$$KL(f:g) = \int f(x) \log \frac{f(x)}{g(x)} dx \ge -\log \int f(x) \frac{g(x)}{f(x)} dx = 0,$$

so KL divergence defines an (asymmetric) distance measure between probability distributions.

Expected and marginal log-likelihood

Since $f(x | y; \theta) = f\{(x, y); \theta\}/f(y; \theta)$ we have

$$q(\theta \mid \theta^*) = \int \log \frac{f(y;\theta)f(x \mid y;\theta)}{f(y;\theta^*)f(x \mid y;\theta^*)} f(x \mid y;\theta^*) dx$$

$$= \log f(y;\theta) - \log f(y;\theta^*)$$

$$+ \int \log \frac{f(x \mid y;\theta)}{f(x \mid y;\theta^*)} f(x \mid y;\theta^*) dx$$

$$= l_y(\theta) - l_y(\theta^*) - KL(f_{\theta^*}^y : f_{\theta}^y).$$

Since the KL-divergence is minimized for $\theta = \theta^*$, differentiation of the above expression yields

$$\frac{\partial}{\partial \theta} q(\theta \,|\, \theta^*) \bigg|_{\theta = 0.5} = \frac{\partial}{\partial \theta} l_y(\theta) \bigg|_{\theta = 0.5}.$$

Let now $\theta_0=\theta^*$ and define the iteration

$$\theta_{n+1} = \arg \max_{\theta} q(\theta \mid \theta_n).$$

Then

$$\begin{array}{lcl} l_y(\theta_{n+1}) & = & l_y(\theta_n) + q(\theta_{n+1} \mid \theta_n) + KL(f^y_{\theta_{n+1}} : f^y_{\theta_n}) \\ & \geq & l_y(\theta_n) + 0 + 0. \end{array}$$

So the log-likelihood never decreases after a combined E-step and M-step.

It follows that any limit point must be a saddle point or a local maximum of the likelihood function.

The picture on the next overhead should show it all.

Expected and complete data likelihood

$$KL(f_{\theta^*}^y:f_{\theta}^y) \ge 0$$

$$V_{\theta^*}$$

$$l_{y}(\theta) - l_{y}(\theta^{*}) = q(\theta \mid \theta^{*}) + KL(f_{\theta^{*}}^{y} : f_{\theta}^{y})$$

$$\nabla l_{y}(\theta^{*}) = \frac{\partial}{\partial \theta} l_{y}(\theta) \Big|_{\theta = \theta^{*}} = \frac{\partial}{\partial \theta} q(\theta \mid \theta^{*}) \Big|_{\theta = \theta^{*}}.$$