

ECM algorithm for two clusters, with constraints on the cluster means and variances, and known data variances.

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We assume that $Y_k \sim N(\psi_{G(k)}, \tau_{G(k)k})$ where $\tau_{G(k)k} = \sigma_k^2 + V_{G(k)}$, and $\Pr[G(k) = g] = \pi_g$ for $g = 0, 1$.

The group membership vector G is regarded as missing data for purposes of the "expectation/conditional maximization" algorithm (ECM).

With a normal approximation, the complete data likelihood per observation k is:

$$\begin{aligned} \Pr[Y_k, G(k) | \psi, V, \pi] &= \Pr[Y_k | G(k)] \cdot \Pr[G(k)] \\ &\propto \exp(-(Y_k - \psi_{G(k)})^2 / 2\tau_{G(k)k}) \cdot (\tau_{G(k)k})^{-1/2} \cdot \pi_{G(k)} \end{aligned}$$

Now suppose that the variances σ_k^2 are known (approximately). Define the free variable $\phi = (\psi_0, \psi_1, \pi_1, V_0, V_1)$, and $\pi_0 = 1 - \pi_1$, and similarly for the current fixed estimate ϕ^* . Following standard calculations, the expectation of the complete-data log likelihood is

$$\begin{aligned} Q(\phi, \phi^*) &= E^* \left(- \sum_k ((Y_k - \psi_{G(k)})^2 / 2\tau_{G(k)k}(V) - 1/2 \log \tau_{G(k)k}(V)) + N_0 \log \pi_0 + N_1 \log \pi_1 \right) \\ &= 1/2 \sum_k \sum_g \pi_{gk}^* \left(-(Y_k - \psi_g)^2 / (\sigma_k^2 + V_g) - \log(\sigma_k^2 + V_g) \right) + N_0^* \log \pi_0 + N_1^* \log \pi_1 \end{aligned}$$

with

$$\frac{\pi_{0k}^*}{\pi_{1k}^*} = \frac{\Pr(Y_k, G(k) = 0 | \psi_0^*, V_0^*, \pi_0^*)}{\Pr(Y_k, G(k) = 1 | \psi_1^*, V_1^*, \pi_1^*)} = \frac{\pi_0^* \exp(-(Y_k - \psi_0^*)^2 / 2(V_0^* + \sigma_k^2)) / \sqrt{V_0^* + \sigma_k^2}}{\pi_1^* \exp(-(Y_k - \psi_1^*)^2 / 2(V_1^* + \sigma_k^2)) / \sqrt{V_1^* + \sigma_k^2}}$$

so that $E^* N_g = \sum_k \pi_{gk}^*$ for $g=0,1$.

To maximize Q , we set its partial derivatives to zero.

$$\partial Q / \partial \psi_g = - \sum_k \pi_{gk}^* \left((Y_k - \psi_g) (\sigma_k^2 + \hat{V}_g)^{-1} \right) = 0$$

and

$$\partial Q / \partial V_g = \frac{1}{2} \sum_k \pi_{gk}^* \left(+ (Y_k - \psi_g)^2 (\sigma_k^2 + V_g)^{-2} - (\sigma_k^2 + V_g)^{-1} \right) = 0$$

We cannot solve these two equations simultaneously. However, fixing $V_g = \hat{V}_g$ we can solve the first:

$$\hat{\psi}_g = \frac{\sum_k \pi_{gk}^* Y_k (\sigma_k^2 + \hat{V}_g)^{-1}}{\sum_k \pi_{gk}^* (\sigma_k^2 + \hat{V}_g)^{-1}}$$

and fixing $\psi_g = \hat{\psi}_g$ we can solve the second:

$$\begin{aligned} \sum_k \pi_{gk}^* ((Y_k - \psi_g)^2 - (\sigma_k^2 + V_g)) &= 0 \\ \sum_k \pi_{gk}^* (Y_k - \psi_g)^2 &= \sum_k \pi_{gk}^* (\sigma_k^2 + V_g) = \sum_k \pi_{gk}^* \sigma_k^2 + N_g^* V_g \\ \hat{V}_g &= \max \left(0, \sum_k \pi_{gk}^* (Y_k - \hat{\psi}_g)^2 - \sum_k \pi_{gk}^* \sigma_k^2 \right) / N_g^* \end{aligned}$$

So in the M step we iterate between these formulas for $\hat{\psi}_g$ and for \hat{V}_g . This constitutes an ECM algorithm.

The ECM context makes it easy to account for constraints. In a mixture of correlation distributions, it may be assumed that $\psi_0 = 0$. We might also want to assume $V_0 = 0$, or at least to test it to see if the variation in the $g=0$ component is due only to noise. These constraints are inserted into the respective formulas.