The EM algorithm and the Laplace Approximation

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The Laplace approximation calls for the computation of second derivatives at the likelihood maximum. When the maximum is found by the EM algorithm, there is a convenient way to compute these derivatives. The likelihood gradient can be obtained from the EM-auxiliary, while the Hessian can be obtained from this gradient with the Pearlmutter trick.

1 The Laplace approximation

Let $X$ denote the observed data, $H$ some hidden variables and $\Theta$ the model parameters. We assume the joint distribution:

$$P(X, H, \Theta) = P(X|H, \Theta)P(H|\Theta)P(\Theta)$$

is easy to work with, while the marginal distribution:

$$P(X, \Theta) = \int P(X, H, \Theta) dH$$

has a more complex form. The Laplace approximation calls for finding the mode and Hessian, w.r.t. $\Theta$:

$$\hat{\Theta} = \arg \max P(X, \Theta), \quad \text{and} \quad \Lambda = \nabla^2 \log P(X, \hat{\Theta})$$

The approximation is:

$$P(\Theta|X) \approx \mathcal{N}(\Theta|\hat{\Theta}, -\Lambda^{-1})$$

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1 All integrals are definite integrals, with fixed boundaries. If $H$ is discrete, the integral can be replaced by summation.

2 See: Christopher M. Bishop, *Pattern Recognition and Machine Learning* (Information Science and Statistics), Springer, 2007; David J. C. MacKay, *Information Theory, Inference, and Learning Algorithms*, Cambridge University Press, 2003.
2 EM-algorithm

If we are using the EM-algorithm for finding the maximum, \( \hat{\Theta} \), then the EM-auxiliary provides a convenient route to the Hessian.

2.1 The EM auxiliary

Let \( \Theta' \) be any valid parameter value satisfying \( \int P(H|X, \Theta') dH = 1 \). We construct the EM auxiliary as follows:

\[
\log P(X, \Theta) = \int P(H|X, \Theta') \log P(X, \Theta) dH
\]

\[
= \int P(H|X, \Theta') \log P(X|\Theta) dH + \log P(\Theta)
\]

\[
= \int P(H|X, \Theta') \log P(X, H|\Theta) P(H|X, \Theta') dH + \log P(\Theta)
\]

\[
= \int P(H|X, \Theta') \log \left[ P(X, H|\Theta) \frac{P(H|X, \Theta)}{P(H|X, \Theta')} \right] dH + \log P(\Theta)
\]

\[
= A(\Theta', \Theta) + D(\Theta', \Theta) \tag{5}
\]

where \( A(\Theta', \Theta) \) is the EM-auxiliary:

\[
A(\Theta', \Theta) = \int P(H|X, \Theta') \log \frac{P(X, H|\Theta)}{P(H|X, \Theta')} dH + \log P(\Theta) \tag{6}
\]

and \( D(\Theta', \Theta) \geq 0 \) is KL-divergence:

\[
D(\Theta', \Theta) = \int P(H|X, \Theta') \log \frac{P(H|X, \Theta')}{P(H|X, \Theta)} dH \tag{7}
\]

Notice that if we zero the divergence by choosing \( \Theta' = \Theta \), then:

\[
\log P(X, \Theta) = A(\theta, \theta) \tag{8}
\]

2.2 Algorithm

Although this note is not about the algorithm itself, we very briefly summarize it. An iteration of the EM-algorithm proceeds as follows: Start at \( \Theta_1 \). The E-step effectively maximizes \( A(\Theta', \Theta_1) \) w.r.t. \( \Theta' \) by simply setting \( \Theta' = \Theta_1 \), which minimizes (and therefore zeros) the divergence.\(^3\) The M-step now

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\(^3\)Here we vary \( \Theta' \), while \( \Theta \) and therefore \( \log P(X, \Theta) \) remain fixed. Then decreasing \( D \) must increase \( A \).
maximizes $A(\Theta_1, \Theta)$, w.r.t. the other parameter, $\Theta$, usually by zeroing partial derivatives. This gives some value $\Theta_2$, such that $A(\Theta_1, \Theta_2) \geq A(\Theta_1, \Theta_1)$. The net effect of both steps is:

$$\log P(X, \Theta_2) = A(\Theta_2, \Theta_2) \geq A(\Theta_1, \Theta_2) \geq A(\Theta_1, \Theta_1) = \log P(X, \Theta_1) \quad (9)$$

### 3 Derivatives

We find the Hessian of $\log P(X, \Theta)$ in two steps. First we find the gradient, which we then differentiate again using the Pearlmutter trick.

#### 3.1 Gradient

The gradient of $\log P(X, \Theta)$ coincides with the gradient of the auxiliary. We show how this works.

Let $\theta$ denote some component of $\Theta$, then, for any value of $\Theta'$, we have:

$$\frac{\partial}{\partial \theta} \log P(X, \Theta) = \frac{\partial}{\partial \theta} A(\Theta', \Theta) + \frac{\partial}{\partial \theta} D(\Theta', \Theta) \quad (10)$$

Note: we are differentiating only w.r.t. the components of $\Theta$ and not w.r.t. those of $\Theta'$. The derivative of the divergence is:

$$\frac{\partial}{\partial \theta} D(\Theta', \Theta) = - \int \frac{P(H|X, \Theta')}{P(H|X, \Theta)} \frac{\partial}{\partial \theta} P(H|X, \Theta) \, dH \quad (11)$$

which conveniently vanishes at $\Theta' = \Theta$:

$$\left[ \frac{\partial}{\partial \theta} D(\Theta', \Theta) \right]_{\Theta' = \Theta} = - \int \frac{\partial}{\partial \theta} P(H|X, \Theta) \, dH$$

$$= - \frac{\partial}{\partial \theta} \int P(H|X, \Theta) \, dH = - \frac{\partial}{\partial \theta} 1 = 0 \quad (12)$$

Putting this together, we find:

$$\frac{\partial}{\partial \theta} \log P(X, \Theta) = \left[ \frac{\partial}{\partial \theta} A(\Theta', \Theta) \right]_{\Theta' = \Theta}$$

$$= \int P(H|X, \Theta) \frac{\partial}{\partial \theta} \log P(X, H, \Theta) \, dH \quad (13)$$

For exponential family distributions, the RHS is usually more convenient than the LHS, because now the log directly simplifies $P(X, H, \Theta)$. Also note that it is unnecessary to differentiate the posterior $P(H|X, \Theta)$, or any associated entropy or divergence.
3.1.1 Other derivatives

Just for interest, we mention here that there are two other derivatives that also vanish:

\[
\left[ \frac{\partial}{\partial \theta'} A(\Theta', \Theta) \right]_{\Theta' = \Theta} = \left[ \frac{\partial}{\partial \theta'} D(\Theta', \Theta) \right]_{\Theta' = \Theta} = 0 \tag{14}
\]

where \( \theta' \) is any component of \( \Theta' \). This is because at \( \Theta' = \Theta \), \( A \) is maximized w.r.t. \( \Theta' \), while \( D \) is minimized w.r.t. both arguments. Only \( \frac{\partial}{\partial \theta} A \) does not vanish here, because it is not necessarily at the maximum w.r.t. \( \Theta \).

3.2 Hessian

We first examine the Hessian analytically. We now consider \( \theta_i, \theta_j \), both components of \( \Theta \) and differentiate first w.r.t. the one and then the other:

\[
\frac{\partial^2}{\partial \theta_i \partial \theta_j} \log P(X, \Theta) = \frac{\partial}{\partial \theta_j} \int P(H|X, \Theta) \frac{\partial^2}{\partial \theta_i \partial \theta_j} \log P(X, H, \Theta) dH = \int P(H|X, \Theta) \frac{\partial^2}{\partial \theta_i \partial \theta_j} \log P(X, H, \Theta) dH + \int \frac{\partial}{\partial \theta_j} P(H|X, \Theta) \frac{\partial}{\partial \theta_i} \log P(X, H, \Theta) dH = \left[ \frac{\partial^2}{\partial \theta_i \partial \theta_j} A(\Theta', \Theta) \right]_{\Theta' = \Theta} + \int \frac{\partial}{\partial \theta_j} P(H|X, \Theta) \frac{\partial}{\partial \theta_i} \log P(X, H, \Theta) dH \tag{15}
\]

This is the Hessian of the auxiliary plus an extra term that can get messy to derive and implement. The Pearlmutter trick gives a convenient alternative:

3.2.1 Pearlmutter trick

Let \( \nabla f(\Theta) \), a column vector, denote the gradient of some multivariate function \( f \), evaluated at \( \Theta \). Similarly, let \( \nabla^2 f(\Theta) \), a square matrix, denote the Hessian. Then the Pearlmutter trick\(^4\) computes the product of the Hessian with an arbitrary column vector, \( v \), as:

\[
\nabla^2 f(\Theta)v = \left[ \frac{\partial}{\partial \alpha} \nabla f(\Theta + \alpha v) \right]_{\alpha = 0} \tag{16}
\]

\(^4\)Barak A. Pearlmutter, “Fast exact multiplication by the Hessian”, Neural Computation, vol. 6, pp. 147160, 1994.
When $\Theta$ has $n$ components, the trick must be applied $n$ times, to map out the columns of the Hessian by successively choosing $v = [1, 0, 0, \ldots]$, $v = [0, 1, 0, \ldots]$ and so on.

For practical implementation, the gradient using (13) could be derived\(^5\) and coded by hand. When that function is available, the differentiation could be done via forward-mode, algorithmic differentiation. If complex arithmetic is available, then that can be done with minimal coding effort via complex-step differentiation.

\(^5\)The M-step should be based on those same derivatives.