

The Expectation-Maximization (EM) Algorithm

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$$\log p(x; \theta) = \log \sum_z p(z, x; \theta) = \log \sum_z q(z) \frac{p(z, x; \theta)}{q(z)} \geq \sum_z q(z) \log p(x, z; \theta) - \sum_z q(z) \log q(z) = F(\theta, q)$$

$F(\theta, q)$ is called Evidence Lower BOund (ELBO) or negative free energy.

$$\begin{aligned} \log p(x; \theta) - F(\theta, q) &= \sum_z q(z) \log \frac{q(z)}{p(z|x; \theta)} = KL(q(z) || p(z|x; \theta)) \\ \Rightarrow \log p(x; \theta) &= F(\theta, p(z|x; \theta)) = \max_q F(\theta, q) \end{aligned}$$

$$\Rightarrow \theta_{ML} = \arg \max_{\theta} \log p(x; \theta) = \arg \max_{\theta} \max_q F(\theta, q)$$

Iterative EM algorithm:

- E-step: $q(z) = p(z|x; \theta_0)$
- M-step: $\theta_1 = \arg \max_{\theta} Q(\theta, \theta_0)$ s.t. $Q(\theta, \theta_0) = \sum_z p(z|x; \theta_0) \log p(x, z; \theta)$ is the auxiliary function:

Theorem: $p(x; \theta_1) \geq p(x; \theta_0)$

Variational EM:

$$\log p(x; \theta) = \log \sum_z p(z, x; \theta) \geq \sum_z q(z|x; \lambda) \log p(x, z; \theta) - \sum_z q(z|x; \lambda) \log q(z|x; \lambda) = F(\theta, \lambda)$$

$$\log p(x; \theta) - F(\theta, \lambda) = \sum_z q(z|x; \lambda) \log \frac{q(z|x; \lambda)}{p(z|x; \theta)} = KL(q(z|x; \lambda) || p(z|x; \theta))$$

$F(\theta, \lambda)$ is called Evidence Lower BOund (ELBO) or negative free energy. The ELBO score can be also written as:

$$F(\theta, \lambda) = \sum_z q(z|x; \lambda) \log p(x, z; \theta) - KL(q(z|x; \lambda) || p(z; \theta))$$

$$\hat{\theta} = \arg \max_{\theta} \log p(x; \theta) = \arg \max_{\theta} \max_{\lambda} F(\theta, \lambda) \geq \arg \max_{\theta} \max_{\lambda \in \Lambda} F(\theta, \lambda)$$

E-step: Find $\lambda \in \Lambda$ that maximizes $F(\theta, \lambda)$.

M-step: Find θ that maximizes $\sum_z q(z|x; \lambda) \log p(x, z; \theta)$.