Two Pages on the EM Algorithm

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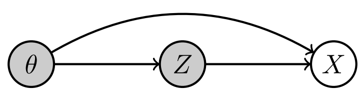
Suppose we observe a realization of the random variable X drawn from some distributions P_θ with an unknown parameter θ; we then want to solve the maximum likelihood problem

$$\max_\theta \quad \log P_\theta(X).$$

Such a problem can be complicated by the presence of an unobserved nuisance variable Z whose joint distribution with X depends on θ:



Examples of such nuisance variables include:

- the syntactic tree Z that generated an observed sentence X
- the chain of hidden states Z that generated a sequence of observations X
- the identities Z of the mixture components that generated the observations in a sample X from a mixture model

We can marginalize the nuisance variable out of the model by integrating the joint probabilities $P_\theta(X \mid Z)\, P_\theta(Z)$ over Z, i.e., taking the expectation of $P_\theta(X \mid Z)$ with respect to the marginal distribution $P_\theta(Z)$. We can therefore formulate the maximum likelihood problem with a nuisance variable as

$$\max_\theta \quad \log E_{Z\sim P_\theta}\left[P_\theta(X \mid Z)\right].$$

Unfortunately, the only way of computing the expectation $E_{Z\sim P_\theta}\left[P_\theta(X \mid Z)\right]$ is usually to enumerate all possible values of Z, and this is often prohibitively expensive. We therefore introduce the surrogate reward function

$$R(\theta, Q) \;=\; E_{Z\sim Q}\left[\log \frac{P_\theta(X, Z)}{Q(Z)}\right].$$

Since this is the expectation of a logarithm, we can often break it up into a sum of expectations whose terms are easier to evaluate. We can then use the equation $E[A+B] = E[A]+E[B]$, which is valid for dependent random variables too, to add up those simpler terms.

By Jensen's inequality, Kullback-Leibler divergences are positive,

$$E_Q\left[\log\frac{Q}{P}\right] \geq 0,$$

with equality if and only if $P = Q$. Hence

$$R(\theta, Q) \;=\; \log P_\theta(X) \;-\; \underbrace{E_{Z\sim Q}\left[\log\frac{Q(Z)}{P_\theta(Z\,|\,X)}\right]}_{\text{KL divergence}} \;\leq\; \log P_\theta(X).$$

The surrogate reward is therefore a lower bound on the true reward. This bound holds with equality if and only if Q is the conditional distribution of Z given X and θ.

In fact, the gap between $R(\theta, Q)$ and $\log P_\theta(X)$ is exactly the Kullback-Leibler divergence from $Q(Z)$ to $P_\theta(Z\,|\,X)$. For a fixed θ, there is thus a unique distribution Q_θ that maximizes $R(\theta, Q)$, namely the conditional distribution

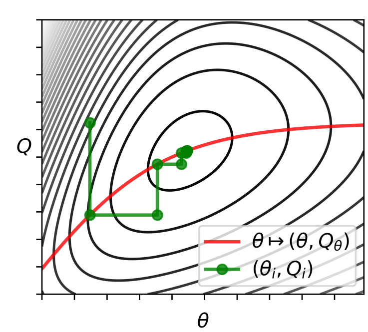
$$Q_\theta(Z) \;=\; P_\theta(Z\,|\,X).$$

All maxima of $R(\theta, Q)$ therefore occur at points of the form (θ, Q_θ). At such points, the KL divergence vanishes, and the surrogate reward is equal to the true reward. Consequently, if a pair (θ^*, Q^*) maximizes the surrogate reward, then θ^* maximizes the true reward.

We can solve the surrogate problem by coordinate ascent. This involves picking an arbitrary initial value (θ_0, Q_0) and then repeating the steps

$$\begin{aligned} Q_{i+1} \quad &\longleftarrow \quad \max_Q \; R(\theta_i, Q) \\ \theta_{i+1} \quad &\longleftarrow \quad \max_\theta \; R(\theta, Q_{i+1}) \end{aligned}$$

until improvement slows down. Since both of these steps are maximizations, they cannot decrease the value of the surrogate reward; the process either has to get stuck or converge to a local maximum.



We have seen that the optimal value of Q_{i+1} given θ_i is the conditional distribution of Z given X. As for the optimal θ_{i+1} given Q_{i+1}, we can write

$$R(\theta, Q) \;=\; E_{Z\sim Q}\left[\log P_\theta(X, Z)\right] \;-\; \underbrace{E_{Z\sim Q}\left[\log Q(Z)\right]}_{\text{entropy of } Q}.$$

Since the entropy of Q is independent of θ, we can compute θ_{i+1} by solving

$$\max_\theta \; E_{Z\sim Q_{i+1}}\left[\log P_\theta(X, Z)\right].$$

For the reasons mentioned above, this expectation can frequently be broken up into a sum of differentiable terms which are reasonably easy to optimize.