EM algorithm

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Latent variables ML

Suppose objects have observed features x and unobserved (latent) features z[1].

- $[x, z] \sim p(x, z, \theta)$, $x \sim p(x, \theta)$
- denote $X = [x_1, x_2, ...x_N]$, $Z = [z_1, z_2, ...z_N]$.

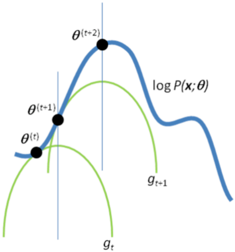
To find $\widehat{\theta}$ we need to solve

$$L(\theta) = \ln p(X|\theta) = \ln \sum_Z p(X, Z|\theta) \to \max_\theta$$

- This is intractable for unknown Z.
- We need to fallback to iterative optimization, such as SGD.
- Alternatively, we may use EM algorithm, which "averages" over different fixed variants of Z.

[1] They are considered discrete here. Everything holds true for continious latent variables if everywhere you replace summation over Z with integration

General idea of EM algorithm



- Initialize $\widehat{\theta}_0$ randomly, $t = 0$
- Repeat until convergence:
  1. $g_t(\theta)$ is estimated as lower bound for $\ln p(X|\theta)$, tight for $\widehat{\theta}_t$
  2. $\widehat{\theta}_{t+1} = \arg\max_\theta g_t(\theta)$
  3. $t = t + 1$

Distribution of latent variables

Let's introduce $q(Z)$ - some distribution over latent variables Z, $q(Z) \geq 0$, $\sum_Z q(Z) = 1$. Then

$$\begin{aligned} L(\theta) = \ln p(X|\theta) &= \ln \sum_Z p(X, Z|\theta) \\ &= \ln \sum_Z q(Z) \frac{p(X, Z|\theta)}{q(Z)} \quad (1) \\ &\geq \sum_Z q(Z) \ln \frac{p(X, Z|\theta)}{q(Z)} = g(\theta) \quad (2) \end{aligned}$$

On the last step we used Jensen's inequality $\ln(\mathbb{E}u_n) \geq \mathbb{E}(\ln u_n)$ applied to

1. $\ln x$ which is strictly concave, because $(\ln x)'' = -\frac{1}{x^2} < 0$
2. for r.v. $U \in \mathbb{R}$ with distribution $p\left(U = \frac{p(X,Z,\theta)}{q(Z)}\right) = q(Z)$ for different Z.

Making lower bound tight

We can select $q(Z)$ so that at fixed θ $L(\theta) = g(\theta)$:

- Since $\ln x$ is strictly concave, equality in inequality (1)-(2) is achieved <=> $U = \mathbb{E}U$ with probability 1.
- This happens when $\frac{p(X,Z|\theta)}{q(Z)} = c$ for some constant c $\forall Z$.
- Using property $\sum_Z q(Z) = 1$ we have

$$c \sum_Z q(Z) = c = \sum_Z p(X, Z|\theta) = p(X|\theta)$$

- So for lower bound $g(\theta)$ to be tight at θ, we need to take

$$q(Z) = \frac{p(X, Z|\theta)}{p(X|\theta)} = p(Z|X, \theta)$$

EM algorithm

INPUT:

training set $X = [x_1, ...x_N]$

some initialization **for** $\hat{\theta}$

some predefined convergence criteria

ALGORITHM:

$t = 0$, θ_0 - init randomly

repeat until convergence:

E-step: set distribution over latent variables:

$$q(Z) = p(Z|X, \hat{\theta}_t)$$

M-step: improve estimate of θ:

$$\hat{\theta}_{t+1} = \arg\max_\theta \{\sum_Z q(Z) \ln \frac{p(X, Z|\theta)}{q(Z)}\}$$

$$t = t + 1$$

OUTPUT:

ML estimate $\hat{\theta}_{t+1}$ **for** the training set.

Equivalent M-step

M-step can be equivalently represented as

$$
\begin{aligned}
\hat{\theta}_{t+1} &= \arg\max_{\theta}\{\sum_{Z} q(Z)\ln\frac{p(X,Z|\theta)}{q(Z)}\} \\
&= \arg\max_{\theta}\{\sum_{Z} q(Z)\ln p(X,Z|\theta) - \overbrace{\sum_{Z} q(Z)\ln q(Z)}^{const(\theta)}\} \\
&= \arg\max_{\theta}\{\sum_{Z} q(Z)\ln p(X,Z|\theta)\} \\
&= \arg\max_{\theta}\{\sum_{Z} p(Z|X,\widehat{\theta}_t)\ln p(X,Z|\theta)\} \\
&= \arg\max_{\theta}\{\mathbb{E}_Z\{\ln p(X,Z|\theta)\}, \quad Z \sim q(Z) = p(Z|X,\widehat{\theta}_t)
\end{aligned}
$$

Comments

Theorem 1

EM estimates of θ on each iteration $\widehat{\theta}_1, \widehat{\theta}_2, \widehat{\theta}_3, ...$ lead to non-decreasing sequence of likelihoods $L(\widehat{\theta}_1) \geq L(\widehat{\theta}_2) \geq L(\widehat{\theta}_3) \geq ...$

Proof.

1. Suppose that at iteration t we have $L(\widehat{\theta}_t)$.
2. At the E-step among all lower bounds $g(\theta) \leq L(\theta)\, \forall\theta$ we select such lower bound $g_t(\cdot)$, that $L(\widehat{\theta}_t) = g_t(\widehat{\theta}_t)$ (by selecting $q_n(Z)$).
3. On M-step we find $\widehat{\theta}_{t+1} = \arg\max_\theta g_t(\theta)$, so $g_t(\widehat{\theta}_{t+1}) \geq g_t(\widehat{\theta}_t)$
4. Since $g_t(\cdot)$ is lower bound, we have $L(\widehat{\theta}_{t+1}) \geq g_t(\widehat{\theta}_{t+1}) \geq g_t(\widehat{\theta}_t) = L(\widehat{\theta}_t)$

□

Since $L(\widehat{\theta}_t)$ is non-decreasing and is bounded from above $(L(\theta) \leq \sum_{n=1}^N \ln 1 = 0)$ it converges.

Comments on EM algorithm

- On M-step $q(Z)$ does not depend on θ, since this parameter was taken fixed from E-step.
- Possible convergence criteria:
  - $\left\|\widehat{\theta}_{t+1} - \widehat{\theta}_t\right\| < \varepsilon$
  - $L(\widehat{\theta}_{t+1}) - L(\widehat{\theta}_t) < \varepsilon$
  - maximum number of iterations reached
- EM converges to local optimum
  - to improve quality it is good to
    - re-run algorithm from different initial conditions
    - select estimate that gives the greatest likelihood
- To guarantee convergence it is not required to solve $\widehat{\theta}_{t+1} = \arg\max_\theta g_t(\theta)$ precisely.
  - we can make very coarse (e.g. single step) optimization here
  - this is called GEM algorithm (generalized EM)

Comments on EM algorithm

- EM can also be applied for MAP optimization
- Define $J(Q,\theta)=\sum_Z q(Z)\ln\frac{p(X,Z|\theta)}{q(Z)}$.
- We know that $L(\theta)\ge J(Q,\theta)$ for all $Q=Q(Z)$.
- EM algorithm can be viewed as coordinate ascent:
    - E-step maximizes $J(Q,\theta)$ w.r.t. Q[2]
    - M-step maximizes $J(Q,\theta)$ w.r.t. θ

[2] We know that, because we chose such Q that ensure equality in Jensen's inequality.

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Independent observations

- Consider special case, when (x_n, z_n) are i.i.d.[3]
  - Examples:.
    - z_n is unknown mixture component, generating x_n
    - z_n are missing variables in i.i.d. x_n
- **E-step** becomes:

$$q(Z) = p(Z|X,\theta) = p(z_1|x_1,\theta)...p(z_N|x_N,\theta) = q_1(z_1)...q_N(z_N)$$

for

$$q_n(z_n) = p(z_n|x_n,\theta)$$

[3] i.i.d.=independent and identically distributed.

Independent observations

- **M-step** becomes:

$$
\begin{aligned}
\hat{\theta} &= \arg\max_{\theta}\{\sum_{Z} q(Z)\ln p(X,Z|\theta)\} \\
&= \arg\max_{\theta}\{\sum_{Z} q(Z)\sum_{n=1}^{N}\ln p(x_n,z_n|\theta)\} \\
&= \arg\max_{\theta}\{\sum_{n=1}^{N}\sum_{z_1,\dots z_N} q(z_1,\dots z_N)\ln p(x_n,z_n|\theta)\} \\
&= \arg\max_{\theta}\{\sum_{n=1}^{N}\sum_{z_1,\dots z_N} q_1(z_1)\dots q_N(z_N)\ln p(x_n,z_n|\theta)\} \\
&= \arg\max_{\theta}\{\sum_{n=1}^{N}\sum_{z_n} q_n(z_n)\ln p(x_n,z_n|\theta)\}
\end{aligned}
$$

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Distribution of latent variables-MAP estimate

Consider r.v. θ with prior distribution $\theta \sim p(\theta)$. A prosteriori likelihood:

$$\begin{aligned}
L(\theta) = \ln p(\theta) + \ln p(X|\theta) = \ln p(X,\theta) = \ln \sum_Z p(X,Z,\theta) \\
= \ln \sum_Z q(Z) \frac{p(X,Z,\theta)}{q(Z)} \qquad (3) \\
\geq \sum_Z q(Z) \ln \frac{p(X,Z,\theta)}{q(Z)} = \sum_Z q(Z) \ln \frac{p(X,Z|\theta)p(\theta)}{q(Z)} \qquad (4) \\
= \sum_Z q(Z) \ln p(X,Z|\theta) + \ln p(\theta) - \underbrace{\sum_Z q(Z) \ln q(Z)}_{const(\theta)} = g(\theta) \qquad (5)
\end{aligned}$$

Once again here we used Yensen's inequality.

Making lower bound tight-MAP estimate

We can select $q(Z)$ so that at fixed θ $L(\theta)=g(\theta)$:

- Since $\ln x$ is strictly concave, equality in inequality (3)-(4) is achieved <=> $U=\mathbb{E}U$ with probability 1.
- This happens when $\frac{p(X,Z,\theta)}{q(Z)}=c$ for some constant c $\forall Z$.
- Using property $\sum_Z q(Z)=1$ we have

$$c\sum_Z q(Z)=c=\sum_Z p(X,Z,\theta)=p(X,\theta)$$

- So for lower bound $g(\theta)$ to be tight at θ, we need to take

$$q(Z)=\frac{p(X,Z,\theta)}{p(X,\theta)}=p(Z|X,\theta)$$

EM algorithm - MAP

INPUT:

training set $X = [x_1, ...x_N]$

some initialization **for** $\hat{\theta}$

some predefined convergence criteria

ALGORITHM:

$t = 0$, $\hat{\theta}_0$ - init randomly

repeat until convergence:

E-step: set distribution over latent variables:

$$q(Z) = p(Z|X, \hat{\theta}_t)$$

M-step: improve estimate of θ

$$\hat{\theta}_{t+1} = \arg\max_\theta \{\sum_Z q(Z) \ln \frac{p(X,Z|\theta)}{q(Z)} + \ln p(\theta)\}$$

$$t = t + 1$$

OUTPUT:

ML estimates $\hat{\theta}_{t+1}$ **for** the training set.