CS 2750 Machine Learning
Lecture 15

Expectation Maximization (EM)

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Learning probability distribution

Basic learning settings:

- A set of random variables $\mathbf{X} = \{X_1, X_2, \ldots, X_n\}$
- **A model of the distribution** over variables in $\boldsymbol{X}$ with parameters Θ
- **Data** $D = \{D_1, D_2, .., D_N\}$

  s.t. $D_i = (x_1^i, x_2^i, \ldots x_n^i)$

Objective: find parameters $\hat{\Theta}$ that describe the data

Assumptions considered so far:

- Known parameterizations
- No hidden variables
- No-missing values

Hidden variables

Modeling assumption:

Variables $\mathbf{X} = \{X_1, X_2, \ldots, X_n\}$

- Additional variables are hidden – never observed in data

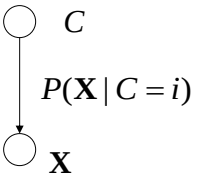
Why to add hidden variables?

- **More flexibility in describing the distribution** $P(\mathbf{X})$
- **Smaller parameterization of** $P(\mathbf{X})$
  - **New independences can be introduced via hidden variables**

Example:

- Latent variable models
  - hidden classes (categories)

Hidden class variable



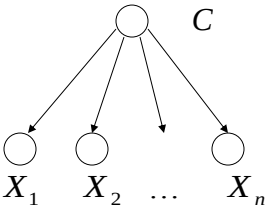
Naïve Bayes with a hidden class variable

Introduction of a hidden variable can reduce the number of parameters defining $P(\mathbf{X})$

Example:

- Naïve Bayes model with a hidden class variable

Hidden class variable



Attributes are independent given the class

- **Useful in customer profiles**
  - Class value = type of customers

Missing values

A set of random variables $\mathbf{X} = \{X_1, X_2, \ldots, X_n\}$

- **Data** $D = \{D_1, D_2, .., D_N\}$
- **But some values are missing**

$$D_i = (x_1^i, x_3^i, \ldots x_n^i)$$

Missing value of x_2^i

$$D_{i+1} = (x_3^{i+1}, \ldots x_n^{i+1})$$

Missing values of x_1^{i+1}, x_2^{i+1}

Etc.

- **Example: medical records**
- **We still want to estimate parameters of** $P(\mathbf{X})$

Density estimation

Goal: Find the set of parameters $\hat{\Theta}$

Estimation criteria:

- **ML** $\max_{\Theta} p(D \mid \Theta, \xi)$
- **Bayesian** $p(\Theta \mid D, \xi)$

Optimization methods for ML: gradient-ascent, conjugate gradient, Newton-Rhapson, etc.

Problem: No or very small advantage from the structure of the corresponding belief network when there are unobserved values

Expectation-maximization (EM) method

- An alternative optimization method
- Suitable when there are missing or hidden values
- **Takes advantage of the structure of the belief network**

General EM

The key idea of a method:

Compute the parameter estimates iteratively by performing the following two steps:

Two steps of the EM:

1. **Expectation step**. For all hidden and missing variables (and their possible value assignments) calculate their expectations for the current set of parameters Θ'
2. **Maximization step**. Compute the new estimates of Θ by considering the expectations of the different value completions

Stop when no improvement possible

EM

Let H – be a set of hidden or missing variable values

Derivation

$$P(H, D \mid \Theta, \xi) = P(H \mid D, \Theta, \xi) P(D \mid \Theta, \xi)$$

$$\log P(H, D \mid \Theta, \xi) = \log P(H \mid D, \Theta, \xi) + \log P(D \mid \Theta, \xi)$$

$$\log P(D \mid \Theta, \xi) = \log P(H, D \mid \Theta, \xi) - \log P(H \mid D, \Theta, \xi)$$

Log-likelihood of data

Average both sides with $P(H \mid D, \Theta', \xi)$ **for some** Θ'

$$E_{H|D,\Theta'} \log P(D \mid \Theta, \xi) = E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi) - E_{H|D,\Theta'} \log P(H \mid \Theta, \xi)$$

$$\log P(D \mid \Theta, \xi) = Q(\Theta \mid \Theta') + H(\Theta \mid \Theta')$$

Log-likelihood of data

EM algorithm

Algorithm (general formulation)

Initialize parameters Θ

Repeat

Set $\Theta' = \Theta$

1. **Expectation step**
$$Q(\Theta \mid \Theta') = E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi)$$
2. **Maximization step**
$$\Theta = \arg\max_{\Theta} Q(\Theta \mid \Theta')$$

until no or small improvement in Θ $(\Theta = \Theta')$

Questions: Why this leads to the ML estimate ?

What is the advantage of the algorithm?

EM algorithm

- Why is the EM algorithm correct?
- **Claim: maximizing Q improves the log-likelihood**

$$l(\Theta) = Q(\Theta \mid \Theta') + H(\Theta \mid \Theta')$$

Difference in log-likelihoods (current and next step)

$$l(\Theta) - l(\Theta') = Q(\Theta \mid \Theta') - Q(\Theta' \mid \Theta') + H(\Theta \mid \Theta') - H(\Theta' \mid \Theta')$$

Subexpression $H(\Theta \mid \Theta') - H(\Theta' \mid \Theta') \geq 0$

Kullback-Leibler (KL) divergence (distance between 2 distributions)

$$KL(P \mid R) = \sum_i P_i \log \frac{P_i}{R_i} \geq 0$$ Is always positive !!!

$$H(\Theta \mid \Theta') = -E_{H|D,\Theta'} \log P(H \mid \Theta, D, \xi) = -\sum_i p(H \mid D, \Theta') \log P(H \mid \Theta, D, \xi)$$

$$H(\Theta \mid \Theta') - H(\Theta' \mid \Theta') = \sum_i P(H \mid D, \Theta') \log \frac{P(H \mid \Theta', D, \xi)}{P(H \mid \Theta, D, \xi)} \geq 0$$

EM algorithm

Difference in log-likelihoods

$$l(\Theta) - l(\Theta') = Q(\Theta \mid \Theta') - Q(\Theta' \mid \Theta') + H(\Theta \mid \Theta') - H(\Theta' \mid \Theta')$$

$$l(\Theta) - l(\Theta') \geq Q(\Theta \mid \Theta') - Q(\Theta' \mid \Theta')$$

Thus

by **maximizing Q we maximize the log-likelihood**

$$l(\Theta) = Q(\Theta \mid \Theta') + H(\Theta \mid \Theta')$$

EM is a first-order optimization procedure

- **Climbs the gradient**
- **Automatic learning rate**

No need to adjust the learning rate !!!!

EM advantages

Key advantages:

- In many problems (e.g. Bayesian belief networks)

$$Q(\Theta \mid \Theta') = E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi)$$

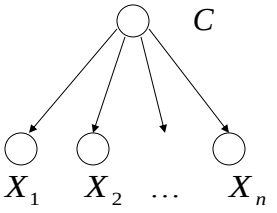
  - has a nice form and the maximization of Q can be carried out in the closed form
- No need to compute Q before maximizing
- We directly optimize
  - using quantities corresponding to expected counts

Naïve Bayes with a hidden class and missing values

Assume:

- $P(\mathbf{X})$ is modeled using a Naïve Bayes model with hidden class variable
- Missing entries (values) for attributes in the dataset D

Hidden class variable



Attributes are independent given the class

EM for the Naïve Bayes

- **We can use EM to learn the parameters**

$$Q(\Theta \mid \Theta') = E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi)$$

- **Parameters:**

π_j prior on class j

θ_{ijk} probability of an attribute i having value k given class j

- **Indicator variables:**

δ_j^l for example *l*, the class is *j* ; if true (=1) else false (=0)

δ_{ijk}^l for example *l*, the class is *j* and the value of attrib *i* is *k*

- because the class is hidden and some attributes are missing, the values (0,1) of indicator variables are not known; they are hidden

H – a collection of all indicator variables

EM for the Naïve Bayes model

- We can use EM to do the learning of parameters

$$Q(\Theta \mid \Theta') = E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi)$$

$$\log P(H, D \mid \Theta, \xi) = \log \prod_{l=1}^{N} \prod_{j} \pi_j^{\delta_j^l} \prod_{i} \prod_{k} \theta_{ijk}^{\delta_{ijk}^l}$$

$$= \sum_{l=1}^{N} \sum_{j} (\delta_j^l \log \pi_j + \sum_{i} \sum_{k} \delta_{ijk}^l \log \theta_{ijk})$$

$$E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi) = \sum_{l=1}^{N} \sum_{j} (E_{H|D,\Theta'}(\delta_j^l) \log \pi_j + \sum_{i} \sum_{k} E_{H|D,\Theta'}(\delta_{ijk}^l) \log \theta_{ijk})$$

$$E_{H|D,\Theta'}(\delta_j^l) = p(C_l = j \mid D_l, \Theta')$$

$$E_{H|D,\Theta'}(\delta_{ijk}^l) = p(X_{il} = k, C_l = j \mid D_l, \Theta')$$

Substitutes 0,1 with expected value

EM for the Naïve Bayes model

- Computing derivatives of ***Q*** for parameters and setting it to 0 we get:

$$\pi_j = \frac{\tilde{N}_j}{N} \qquad \theta_{ijk} = \frac{\tilde{N}_{ijk}}{\sum_{k=1}^{r_i} \tilde{N}_{ijk}}$$

$$\tilde{N}_j = \sum_{l=1}^{N} E_{H|D,\Theta'}(\delta_j^l) = \sum_{l=1}^{N} p(C_l = j \mid D_l, \Theta')$$

$$\tilde{N}_{ijk} = \sum_{l=1}^{N} E_{H|D,\Theta'}(\delta_{ijk}^l) = \sum_{l=1}^{N} p(X_{il} = k, C_l = j \mid D_l, \Theta')$$

- **Important:**
  - **Use expected counts instead of counts !!!**
  - Re-estimate the parameters using expected counts

EM for BBNs

- The same result applies to learning of parameters of **any Bayesian belief network** with discrete-valued variables

$$Q(\Theta \mid \Theta') = E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi)$$

$$\theta_{ijk} = \frac{\tilde{N}_{ijk}}{\sum_{k=1}^{r_i} \tilde{N}_{ijk}} \longleftarrow \text{Parameter value maximizing } \boldsymbol{Q}$$

$$\tilde{N}_{ijk} = \sum_{l=1}^{N} p(x_i^{\,l} = k, pa_i^{\,l} = j \mid D^l, \Theta')$$

may require inference

- **Again:**
  - Use expected counts instead of counts