CMSC828G Principles of Data Mining Lecture #10

- Today's Reading:
  - HMS, 9.6, 6.4, 7.3.2, 7.4, 8.4
- Today's Lecture:
  - Probabilistic Model-based Clustering
  - Descriptive Modeling
- Upcoming Due Dates:
  - H2 due Thu 3/7

Families of Clustering Algorithms

- Partition-based methods
  - e.g., K-means
- Hierarchical clustering
  - e.g., hierarchical agglomerative clustering
- Probabilistic model-based clustering
  - e.g., mixture models

Probabilistic Model-based Clustering

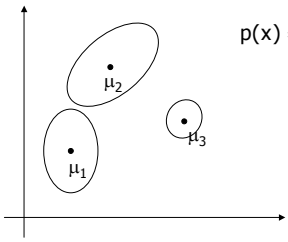
- Assume a probability model for each component cluster
- Mixture Model:

$$f(x) = \sum_{k=1}^{K} w_k f_k(x;\theta_k)$$

- where f_k are component distributions
- components: gaussian, poisson, exponential

Gaussian Mixture Models (GMM)

- K components
- model for each component cluster $N(\mu_k,\sigma_k)$

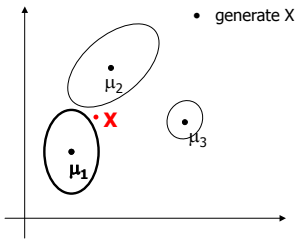


$$p(x) = \sum_{k=1}^{K} w_k f(x;\mu_k,\sigma_k)$$

much borrowed from Andrew Moore's Clustering Gaussian Mixtures Lecture notes

GMM cont.

- Generative Model
  - choose component with probability w_k
  - generate $X \sim N(\mu_k,\sigma_k)$



GMM cont.

- But, we need to learn a model from the data…
- $D = \{x(1), \ldots, x(n)\}$

First, suppose we know $w_1, \ldots, w_k$
$P(x \mid w_j, \mu_1, \ldots, \mu_k, \sigma_1, \ldots, \sigma_k) = ?$

Next,
$P(x \mid \mu_1, \ldots, \mu_k, \sigma_1, \ldots, \sigma_k) = ?$

And,
$P(D \mid \mu_1, \ldots, \mu_k, \sigma_1, \ldots, \sigma_k) = ?$

Look Familiar?

- $P(D \mid \mu_1, \ldots, \mu_k, \sigma_1, \ldots, \sigma_k)$ gives us the probability for a particular choice of $\mu_1, \ldots, \mu_k, \sigma_1, \ldots, \sigma_k$
- How do we choose μ_i σ_i?
- Find μ_i that maximize the likelihood
- Set

$$\frac{\partial}{\partial \mu_j} \log P(D \mid \mu_1, \ldots, \mu_k, \sigma_1, \ldots, \sigma_k) = 0$$

and solve for μ_i

- Problem: we have a bunch on non-linear non-analytically-solvable equations
- One solution: gradient descent…. slow
- instead….

Expectation Maximization (EM)

- Dempster, Laird, and Rubin, 1977
- **extremely** popular recently
- applicable in a wide range of problems
- many uses: hidden markov models,
- basic idea is quite simple…

EM setup

- Let D = {x(1), …, x(n)} be n observed data vectors
- Let H = {z(1),…, z(n)} be n values of hidden variable Z (these might be the cluster labels)
- Then the log-likelihood of the observed data is

$$l(\theta) = \log p(D \mid \theta) = \log \sum_H p(D,H \mid \theta)$$

- *both* θ and H are unknown
- Let Q(H) be any probability distribution for H.

$$\begin{aligned} l(\theta) &= \log \sum_H p(D,H \mid \theta) \\ &= \log \sum_H Q(H) \frac{p(D,H \mid \theta)}{Q(H)} \\ &\geq \sum_H Q(H) \log \frac{p(D,H \mid \theta)}{Q(H)} \\ &= \sum_H Q(H) \log p(D,H \mid \theta) + \sum_H Q(H) \log \frac{1}{Q(H)} \\ &= F(Q,\theta) \end{aligned}$$

lower bound on $l(\theta)$

Jensen's Inequality

- http://www.engineering.usu.edu/classes/ece/7680/lecture2/node5.html

EM Algorithm

- EM algorithm alternates between

Intuition:
·In the E-step, we estimate the distribution on the hidden variables, conditioned on a particular setting of the parameter vector θ^k
·In the M-step, we choose new set of parameters θ^{k+1} to maximize the expected log-likelihood of observed data

- Maximum for E step:

$$Q^{k+1} = p(H \mid D, \theta^k)$$

- Maximum for M step:

$$\theta^{k+1} = \arg \max_{\theta} \sum_H p(H \mid D, \theta^k) \log p(D,H \mid \theta^k)$$

Notes

- Often both the E and M step can be solved in closed form
- Neither the E step nor the M step can decrease the log-likelihood
- Under relatively general conditions the algorithm is guaranteed to converge to a local maximum of log-likelihood
- We must specify a starting point for the algorithm, for example a random choice of θ or Q
- We must specify stopping criteria, or convergence detection
- Computational complexity: number of iterations, time to compute E and M steps

Back to our example…

- We want to fit a normal mixture distribution:

$$f(x) = \sum_{k=1}^{K} w_k f_k(x; \mu_k, \sigma_k)$$

w_k is prior probability of x belonging to component

$\theta = (w_1, \ldots w_k, \mu_1, \ldots, \mu_k, \sigma_1, \ldots, \sigma_k)$ is parameter vector

then probability of data point x coming from kth class is:

E-step: $\hat{P}(k \mid x) = \dfrac{w_k f_k(x; \mu_k, \sigma_k)}{f(x)}$

M-step: $\hat{w}_k = \dfrac{1}{n}\sum_{k=1}^{n} \hat{P}(k \mid x(i))$ $\quad \hat{\mu}_k = \dfrac{1}{n w_k}\sum_{k=1}^{n} \hat{P}(k \mid x(i))x(i)$

$$\hat{\sigma}_k = \frac{1}{n w_k}\sum_{k=1}^{n} \hat{P}(k \mid x(i))(x(i) - \mu_k)^2$$

EM Demo

EM demo

http://diwww.epfl.ch/mantra/tutorial/english/gaussian/html/

EM Comments

- complexity of EM for multivariate gaussian mixtures with K components: dominated by calculation of K covariance matrices.
  - With p dimensions, $O(Kp^2)$ covariance parameters to be estimated
  - Each requires summing over n data points and cluster weights, leading to $O(Kp^2n)$ per step
- Often times there are large increases in likelihood over first few iteration and then can slowly converge; likelihood as function of iterations not necessarily concave

Likelihood as function of EM Iteration

figure 9.2 in text

Probabilistic Model-based clustering

- model provides full distributional description for each component; we may be able to interpret differences in the distributions
- Given the model, each data point has a K-component vector of probabilities that it belongs to each group (why this is called soft-clustering)
- EM algorithm can be extended for MAP and Bayesian estimation
- Method can be extended to data that are not in p dimensional vector form. mixtures of sequence models, e.g. markov models, others
- key cost: assumption of parametric model

and finally…

how do we choose K?

How to choose K

- Choose K that maximizes likelihood?
- NOT.
- As K is increased, the value of the likelihood at maximum cannot decrease
- Problem of scoring models with different complexities

Model Selection

- First, as we mentioned before, there are two possible goals in constructing a model
- Goal #1: summarization
  - we would like to describe the data as precisely as possible
  - given that our model is comprehensible (subjective) or compact (objective)
  - general approach based on data compression and information-theoretic arguments results in a score function:

score(θ,M) = # of bits to describe the data given the model + number of bits to describe the model

$$\text{score}(\theta, M) = \underbrace{-\log p(D \mid \theta, M)}_{\substack{\#\text{ of bits to transmit the data that is not accounted for by the model}}} \underbrace{-\log p(\theta, M)}_{\substack{\#\text{ of bits to transmit the model}}}$$

Model Selection, cont.

- Goal #2: generalize from the available data to new data
  - goodness of fit is part of the objective
  - but, since the data is not the entire population, we want to learn a model that will generalize to other new data instances
- In both cases, we want a score function that strikes a compromise between how well the model fits the data and the simplicity of the model, although the theoretical motivations for this are quite different

Bias-Variance

- Model too flexible $\Rightarrow$ overfit the data $\Rightarrow$ high variance
- Model too restrictive $\Rightarrow$ can't fit the data $\Rightarrow$ high bias
- Bias-variance tradeoff: compromise

Penalize Complexity

- Score(M) = error(M) + penalty-function(M)
- Penalty-function:
  - $M_1, \ldots, M_K$ K models
  - θ_k best parameters
  - complexity of model M depends number of parameters d_k
- AIC - Akaike information criterion:

$$S_{AIC}(M_k) = 2S_L(\hat{\theta}_k; M_k) + 2d_k$$

- BIC – Bayesian information criterion

$$S_{BIC}(M_k) = 2S_L(\hat{\theta}_k; M_k) + d_k \log n$$

- others –Minimum Description Length (MDL), Structural Risk Minimization (SRM)

Bayesian Approach

- compute posterior probability of each model directly and select the one with highest posterior:

$$\begin{aligned} p(M_k \mid D) &\propto p(D \mid M_k)p(M_k) \\ &= \int p(D, \theta_k \mid M_k)p(M_k)d\theta_k \\ &= \int p(D \mid, \theta_k \mid M_k)p(M_k)d\theta_k \end{aligned}$$

implicitly penalizes complexity, since higher dimensional parameter spaces (more complex models) will mean that the probability mass in $p(\theta_k \mid M_K)$ is spread more thinly

often computationally intractable; use MCMC to estimate, use approximation.

External Validation

- General Idea:
  - Split data randomly into two disjoint sets
  - the training set
  - the validation set
  - construct a model based on the training set
  - compute an estimate for the score based on the validation set
  - this estimate for the score will be an unbiased estimate

External Validation, cont.

- popular method: Cross-validation
  - repeatedly split the data into train and validation sets; average results
  - n-fold cross-validation
  - leave one out cross-validation

Summary

- Families of Clustering Algorithms
  - Partition-based methods
  - Hierarchical clustering
  - Probabilistic model-based clustering
- EM Algorithm
- Methods for scoring models with different complexities

Next Time

- Density Estimation
- Reading: ch 9

References

- *Principles of Data Mining*, Hand, Mannila, Smyth. MIT Press, 2001.
- Andrew Moore's excellent lecture notes, http://www-2.cs.cmu.edu/~awm/781/