EECS 445 Final Note

Clustering

Input: $S_n = \{\overline{x}^{(i)}\}_{i=1}^n$ $\overline{x} \in \mathbb{R}^d$

Output: a set of cluster assignments $c_1, \ldots, c_n$, where $c_i \in \{1, \ldots, k\}$

K-means

Datapoints $\overline{x}^{(1)}, \ldots, \overline{x}^{(n)}$ and fixed k. Initial means $\overline{\mu}^{(1)}, \ldots, \overline{\mu}^{(k)}$

Iteratively,

1. reassign $\overline{x}^{(i)}$ to $c_i = \arg\min_j \left\|\overline{x}^{(i)} - \overline{\mu}^{(j)}\right\|^2$
2. recompute $\overline{\mu}^{(j)} = \frac{\sum_i [[c_i=j]]\overline{x}^{(i)}}{\sum_i [[c_i=j]]}$

That is, define $J(\overline{c}, \overline{\mu}) = \sum_{i=1}^n \left\|\overline{x}^{(i)} - \overline{\mu}^{(c_i)}\right\|^2$

First, fix $\overline{\mu}$, choose $\overline{c}$ to minimize J. Second, fix $\overline{c}$, choose $\overline{\mu}$ to minimize J.

k-means performs coordinate descent on the objective function. k-means is guaranteed to converge (because objective function is monotonically decreasing), but not necessarily the global minimum. Solution: vary initialization of k-means, and pick clustering with lowest (eventual) objective function value (for a fixed k).

Spectral Clustering

Weight matrix: W, where w_{ij} represents the similarity between v_i and v_j.

Degree of a vertex: $d_i = \sum_{j=1}^n w_{ij}$

Degree matrix D: $D_{ii} = \sum_{j=1}^n w_{ij}$, $D_{ij} = 0$ for $i \neq j$

Cost of a cut between A and $\overline{A}$: $\text{cut}(A, \overline{A}) = \sum_{i \in A} \sum_{j \in \overline{A}} w_{ij}$

Graph Laplacian: $L = D - W$.

Build matrix with the first k eigenvectors (corresponding to the k smallest eigenvalues) as columns interpret rows as new data points

Apply k-means to new data representation

Hierarchical Clustering

1. Assign each pt. its own cluster, for each point i, $C_i = \{\overline{x}^{(i)}\}$
2. Find the closest clusters & merge, repeat until convergence

$$\arg\min_{i,j} d\left(C_i, C_j\right) \text{ where } i \neq j$$

Recommender Systems

Approach #1: **Nearest Neighbor Prediction**

User: a, b.Y_{ai} is missing, i.e., a has not rated movie i.

Define $R(a, b)$: set of movies rated by both users a and b

$\tilde{Y}_{a:b} = \frac{1}{|R(a,b)|} \sum_{j \in R(a,b)} Y_{a_j}$

$$\text{sim}(a,b) = \frac{\sum_{j \in R(a,b)} \left(Y_{a_j} - \tilde{Y}_{a:b}\right)\left(Y_{b_j} - \tilde{Y}_{b:a}\right)}{\sqrt{\sum_{j \in R(a,b)} \left(Y_{a_j} - \tilde{Y}_{a:b}\right)^2 \sum_{j \in R(a,b)} \left(Y_{b_j} - \tilde{Y}_{b:a}\right)^2}}$$

Define $KNN(a, i)$: k nearest neighbors, i.e., the k most similar users to a, who have rated movie.

$$\hat{Y}_{a_i} = \overline{Y}_a + \frac{1}{\sum_{b \in kNN(a,i)} |\text{sim}(a,b)|} \sum_{b \in kNN(a,i)} \text{sim}(a,b)\left(Y_{b_i} - \overline{Y}_b\right)$$

Approach #2: **Matrix Factorization**

Let $A \in \mathbb{R}^{n \times m}$, and $rank(A) = r$. Then there exists $X \in \mathbb{R}^{n \times r}$, $Y \in \mathbb{R}^{r \times m}$, such that $A = XY$

Given Y with empty cells, construct low rank-d $\widehat{Y}$ with no empty cells. We may think of Y as being approximated by $\widehat{Y} = UV^T$, where $U \in \mathbb{R}^{n \times d}$ contains the relevant features of the user, and $V \in \mathbb{R}^{m \times d}$ contains the relevant features of the movie.

$$J(U,V) = \frac{1}{2} \sum_{(a,i) \in D} (Y_{ai} - [UV^T]_{ai})^2 + \frac{\lambda}{2} \sum_{a=1}^n \sum_{k=1}^d U_{ak}^2 + \frac{\lambda}{2} \sum_{i=1}^m \sum_{k=1}^d V_{ik}^2$$

$U = [\overline{u}^{(1)}, \ldots, \overline{u}^{(n)}]^T$, and $V^T = [\overline{v}^{(1)}, \ldots, \overline{v}^{(m)}]$

Algorithm Overview (coordinate descent)

1. Initialize V to small (random) values.
2. Iterate until convergence

Fix $\overline{v}^{(1)}, \ldots, \overline{v}^{(m)}$. Solve for $\overline{u}^{(1)}, \ldots, \overline{u}^{(n)}$

$$\min_{\overline{u}^{(a)}} \frac{1}{2} \sum_{i \in D_a} (Y_{ai} - \overline{u}^{(a)} \cdot \overline{v}^{(i)})^2 + \frac{\lambda}{2} \|\overline{u}^{(a)}\|^2$$

Fix $\overline{u}^{(1)}, \ldots, \overline{u}^{(n)}$. Solve for $\overline{v}^{(1)}, \ldots, \overline{v}^{(m)}$

$$\min_{\overline{v}^{(i)}} \frac{1}{2} \sum_{a \in D_i} (Y_{ai} - \overline{u}^{(a)} \cdot \overline{v}^{(i)})^2 + \frac{\lambda}{2} \|\overline{v}^{(i)}\|^2$$

i.i.d assumption

Identically drawn from $\mathcal{D}$, each trial independent from each other.

Gaussian Distribution

$$\mathcal{N}\left(x|\mu, \sigma^2\right) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x-\mu)^2}$$

Spherical Gaussian

$$\mathcal{N}\left(\overline{x}|\overline{\mu}, \sigma^2\right) = \frac{1}{(2\pi\sigma^2)^{d/2}} \exp\left(-\frac{1}{2\sigma^2}\|\overline{x} - \overline{\mu}\|^2\right)$$

MLE results

$$\overline{\mu} = \frac{1}{n} \sum_{i=1}^n \overline{x}^{(i)}, \ \sigma^2 = \frac{1}{nd} \sum_{i=1}^n \|\overline{x}^{(i)} - \overline{\mu}\|^2$$

GMM, EM

Iterate until convergence:

E step: use current estimate of mixture model to assign examples to clusters

M step: re-estimate each cluster model separately based on the points assigned to it (similar to the "known cluster" case)

Bayes' Theorem:

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)} = \frac{P(B|A)P(A)}{\sum_A P(B|A)P(A)}$$

E-step: fix parameters $\overline{\theta} = [\gamma_1, \ldots, \gamma_k, \overline{\mu}^{(1)}, \ldots, \overline{\mu}^{(k)}, \sigma_1^2, \ldots, \sigma_k^2]$, compute posterior distribution

$$P(j|i) = \frac{\gamma_i \cdot \mathcal{N}(\overline{x}^{(i)}|\overline{\mu}^{(j)}, \sigma_j^2)}{\sum_{t=1}^k \gamma_t \cdot \mathcal{N}(\overline{x}^{(i)}|\overline{\mu}^{(t)}, \sigma_t^2)}$$

M-step: fix posterior distribution $P(j|i)$, compute MLE parameters $\overline{\theta}$.

$$n_j = \sum_{j=1}^n P(j|i), \quad \gamma_j = \frac{n_j}{n}$$

$$\overline{\mu}^{(j)} = \frac{1}{n_j} \sum_{i=1}^n P(j|i)\overline{x}^{(i)}, \quad \sigma_j^2 = \frac{1}{n_j d} \sum_{i=1}^n P(j|i)\|\overline{x}^{(i)} - \overline{\mu}\|^2$$

EM in general

Bayesian Networks

For a given graph, the joint distribution can be written as a product of the conditional probability of each variable given its parents

$$P\left(X_1, \ldots, X_d\right) = \prod_{i=1}^d P\left(X_i | X_{pa_i}\right)$$

Three Rules

1. $P(X, Y) = P(X|Y)P(Y)$
2. $P(X) = \sum_Y P(X, Y)$
3. $\sum_X P(X|Y) = 1$

d-separation
Step 1: keep only ancestral graph of the variables of interest
Step 2: ("moralize") add undirected edge between any two variables in ancestral graph that have a common child & change to undirected.
Step 3: (i) if there is **no** path between variables of interest, they are marginally independent.
(ii) if **all** paths go through a particular node, then the variables are independent given that node.

MLE learning on Bayesian Networks
log-likelihood: $l(\theta; S_n, G) = \sum_{t=1}^{n} \sum_{i=1}^{d} \log \theta_i(x_i^{(t)}|x_{pai}^{(t)})$
Corresponding MLE:

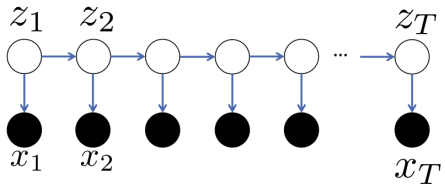
$$\hat{\theta}_i(x_i|x_{pai}) = \frac{\#(X_i = x_i, X_{pai} = x_{pai})}{\sum_{x_i'} \#(X_i = x_i', X_{pai} = x_{pai})}$$

Bayesian Information Criterion, n is number of training data

$$\text{BIC}(D; \overline{\theta}) = l(D; \overline{\theta}) - \frac{\#\,\text{param}}{2} \log(n)$$

M^{th} order Markov Model
Assumption: the t^{th} observation is independent of previous observations given the $(t\text{–}1)^{\text{st}}$,...,$(t\text{–}M)^{\text{th}}$ observations
joint pdf: $P(x_1, \ldots, x_T) = \ldots \Pi_{t=M+1}^{T} P(x_t|x_{t-1}, \ldots, x_{t-M})$
number of parameters: $O(k^{M+1})$

Hidden Markov Model (HMM)
Assumption: the hidden variable (z's) are discrete random variables (x's are observed).



Transition Probabilities: $A(h_i, h_j) = P(z_{t+1} = h_j | z_t = h_i)$
Emission Probabilities: $B(h_i, o_l) = P(x_t = o_l | z_t = h_i)$
Starting State Probability: $\pi(h_i) = P(z_1 = h_i)$
Joint probability distribution: $P(x_1, \ldots, x_T, z_1, \ldots, z_T) = \pi(z_1) \prod_{t=1}^{T-1} A(z_t, z_{t+1}) \prod_{t=1}^{T} B(z_t, x_t)$