

Clusters:

- Kmeans:** (kndt)
- Partition objects into k nonempty subsets
 - Compute seed points as the centroids of the clusters of the current partitioning
 - Assign each object to the cluster with the nearest seed point
 - Go back to Step 2, stop when he assignment does not change
- 随机选取K个质心的值
 - 计算各个点到质心的距离
 - 将点的类别为离他最近的质心，形成K个cluster
 - 根据分类好的cluster，在每个cluster内重新计算质心(平均每个点的值)
 - 重复迭代2-4步直到满足迭代次数或误差小于指定的值

K-Medoids (kndt) : Instead of taking the mean value of the object in a cluster as a reference point(不在内部), medoids can be used, which is the most centrally located object in a cluster. 1、随机选取K个质心的值(质心必须是某些样本点的值，而不是任意值) 2、计算各个点到质心的距离 3、将点的类别分为离他最近的质心，形成K个cluster 4、根据分类好的cluster，在每个cluster内重新计算质心: 4.1 计算cluster内所有样本点到其中一个样本点的曼哈顿距离和(绝对误差) 4.2 选出使cluster绝对误差最小的样本点作为质心 5、重复迭代2-4步直到满足迭代次数或误差小于指定的值

PAM(n^2dt):0. Calculate the pair-wise distance matrix W

- 1.Initialize: randomly select of the data points as the medoids
- 2.Associate each data point to the closest medoid
- 3.For each cluster, compute its medoid
- 4.Repeat 2-3 until there is no change in the medoids (怎么选? 离之心最近的或者 distance row sum 最小的)

GMM:

$$p(x; \Theta) = \sum_{k=1}^K \pi_k p_k(x; \theta_k)$$
$$\Theta = \{\pi_1, \dots, \pi_k, \theta_1, \dots, \theta_k\}, \sum \pi_k = 1$$
$$p_k(x; \theta_k) = \mathcal{N}(x; \mu_k; \Sigma_k)$$

For each point $x^{(i)}$, associate with a hidden variable $z^{(i)}$ denotes which Gaussian $x^{(i)}$ belongs to

Spectral clustering:

Divide vertices into two disjoint groups (A,B). Minimize weight of between-group connections.

$$cut(A,B) = \sum_{i \in A, j \in B} w_{ij}$$
$$assoc(A,V) = \sum_{i \in A, j \in V} w_{ij}$$
$$\min cut(A,B) = \frac{cut(A,B)}{assoc(A,V)} + \frac{cut(A,B)}{assoc(B,V)}$$

Max cluster间的， min cluster之间的

Generalized Eigen-problem

$$\min_y \frac{y^T(D-W)y}{y^T D y}, y \in \mathbb{R}^n, y^T D y = 0$$

Obj of NCut

$$(D-W)y = \lambda D y$$

- Eigenvector corresponding to the **smallest** eigenvalue.
- Vector **1** is the eigenvector corresponding to the eigenvalue 0.
$$(D-W)y = \lambda D^{\frac{1}{2}} D^{\frac{1}{2}} y$$
$$D^{-\frac{1}{2}}(D-W)D^{-\frac{1}{2}} D^{\frac{1}{2}} y = \lambda D^{\frac{1}{2}} y$$
$$D^{-\frac{1}{2}}(D-W)D^{-\frac{1}{2}} x = \lambda x$$

$$x_1^T x_2 = 0 \rightarrow (D^{\frac{1}{2}} x_1)^T (D^{\frac{1}{2}} x_2) = 0 \rightarrow x_1^T D x_2 = 0$$

- The eigenvector corresponding to the **2nd** small eigenvalue.

Spectral Clustering Algorithm

- Graph construction
 - Heat kernel $w_{ij} = \exp\left(-\frac{\|x_i - x_j\|}{2\sigma^2}\right)$
 - k-nearest neighbor graph
- Eigen-problem
 - Compute eigenvalues and eigenvectors of the matrix L
 - Map each point to a lower-dimensional representation based on one or more eigenvectors.
- Conventional clustering schemes, e.g. K-Means
 - Assign points to two or more clusters, based on the new representation.

D = EuDist2(X);
W = (D <= max(mink(D, k+1)));
W = W & (D <= threshold) ;
W = W - eye(size(D)); % clear the distance to itself
W = double(W | W'); % merge the two-direction matrix

D = eye(size(W));
D = D .* sum(W,2);
[Y, ~] = eigs(D - W, D, 2, 'smallestabs');
idx = kmeans(Y(:, 2) k);

- o Perceptron

$$f(x) = w^T x + w_0$$
$$y = \text{sign}(f(x))$$

- o Learn
 - o If correct, do nothing
 - o If wrong, $w_t = w_{t-1} + xy$
- o Perceptron Criterion Function

$$E(w) = - \sum_{i \in IM} w^T x_i y_i$$

- o Gradient Descent (Steepest descent)

$$x_{n+1} = x_n - \gamma \nabla f(x_n), n \geq 0$$

Backpropagation Algorithm

vanishing gradient problem

$$\frac{\partial J}{\partial w_k} = \frac{\partial J}{\partial z} \cdot f'(net_k) \cdot x_k$$
$$\frac{\partial J}{\partial w_3} = \frac{\partial J}{\partial z} \cdot f'(net_4) \cdot w_4 \cdot f'(net_3) \cdot x_3$$
$$\frac{\partial J}{\partial w_2} = \frac{\partial J}{\partial z} \cdot f'(net_4) \cdot w_4 \cdot f'(net_3) \cdot w_3 \cdot f'(net_2) \cdot x_2$$
$$\frac{\partial J}{\partial w_1} = \frac{\partial J}{\partial z} \cdot f'(net_4) \cdot w_4 \cdot f'(net_3) \cdot w_3 \cdot f'(net_2) \cdot w_2 \cdot f'(net_1) \cdot x_1$$

First order derivative

$$J = \frac{1}{2} \sum_{k=1}^c (t_k - x_k)^2$$
$$net_j = \sum_{i=0}^d x_i w_{ji} \quad net_k = \sum_{j=0}^d y_j w_{kj}$$
$$\frac{\partial J}{\partial w_{kj}} = \frac{\partial J}{\partial z_k} \cdot \frac{\partial z_k}{\partial net_k} \cdot \frac{\partial net_k}{\partial w_{kj}} = (z_k - t_k) \cdot f'(net_k) \cdot y_j$$
$$\frac{\partial J}{\partial w_{ji}} = \frac{\partial J}{\partial y_j} \cdot \frac{\partial y_j}{\partial net_j} \cdot \frac{\partial net_j}{\partial w_{ji}} = \left(\sum_{k=1}^c (z_k - t_k) \cdot f'(net_k) \cdot w_{kj} \right) \cdot f'(net_j) \cdot x_i$$

Activation Function

$$f(net) = a \tanh(b \cdot net) = a \left[\frac{1 - e^{-b \cdot net}}{1 + e^{-b \cdot net}} \right] = \frac{2a}{1 + e^{-b \cdot net}} - a$$

The anti-symmetric sigmoid function:
 $f(x) = f(x)$
 $a = 1.718, b = 2/3$.

First order derivative

Activation function: ReLU(x) = max(0, x)

PCA:

Main steps for computing PCs:

- Form the covariance matrix S.
- Compute its eigenvectors: $\{a_i\}_{i=1}^p$
- Use the first d eigenvectors $\{a_i\}_{i=1}^d$ to form the d PCs.
- The transformation A is given by $A = [a_1, \dots, a_d]$

几种常见的数据挖掘算法

- Naïve Bayesian classifier
- Linear Regression
- Logistic Regression
- SVM
- Perceptron
- Neural Network
- k Nearest Neighbor
- Decision Tree

正太分布:

Multivariate density: $N(\mu, \Sigma)$ (with dimension d)

$$P(x) = \frac{1}{(2\pi)^{\frac{d}{2}} |\Sigma|^{\frac{1}{2}}} \exp \left[-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right]$$

- $x = [x_1, \dots, x_d]^T$
- $\mu = [\mu_1, \dots, \mu_d]^T$
- Σ : $d \times d$ covariance matrix, $|\cdot|$: determinant

MLE:

Maximum-Likelihood Estimation

- Use the information in training samples to estimate $\theta = (\theta_1, \theta_2, \dots, \theta_k)$; $\theta_i (i=1, 2, \dots, k)$ is associated with the i -th category
- Suppose sample set D contains n iid samples, x_1, x_2, \dots, x_n
$$p(D|\theta) = \prod_{i=1}^n p(x_i|\theta)$$
- $p(D|\theta)$ is called the likelihood of θ w.r.t. the set of samples.
- ML estimate of θ is, by definition, the value $\hat{\theta}$ that maximizes $p(D|\theta)$
- "It is the value of θ that best agrees with the actually observed training samples"

Bayes Estimation:

- We assume that the true values of the a priori probabilities are known or obtainable from a trivial calculation;
 - We substitute $P(\omega_i) = P(\omega_i|D)$
- Furthermore, we can separate the training samples by class into c subsets D_1, D_2, \dots, D_c , with the samples in D_i belonging to ω_i
$$P(\omega_i|x, D) = \frac{p(x|\omega_i, D_i) P(\omega_i)}{\sum_{j=1}^c p(x|\omega_j, D_j) P(\omega_j)}$$
- In essence, we have c separate problems of the following form: use a set D of samples drawn independently according to the fixed but unknown probability distribution $p(x)$ to determine $P(x|D)$
- This is the central problem of Bayesian learning

Bayesian Parameter Estimation: General Theory

$P(x|\theta)$ computation can be applied to any situation in which the unknown density can be parametrized: the basic assumptions are:

- The form of $P(x|\theta)$ is assumed known, but the value of θ is not known exactly
- Our knowledge about θ is assumed to be contained in a known prior density $P(\theta)$
- The rest of our knowledge about θ is contained in a set D of n random variables x_1, x_2, \dots, x_n that follows $P(x)$

Discriminant Functions for the Normal Density

- The minimum error-rate classification can be achieved by the discriminant function
$$g_i(x) = \ln P(x|\omega_i) + \ln P(\omega_i)$$
- In case of multivariate normal densities
$$P(x|\omega_i) = \frac{1}{(2\pi)^{\frac{d}{2}} |\Sigma_i|^{\frac{1}{2}}} \exp \left[-\frac{1}{2} (x - \mu_i)^T \Sigma_i^{-1} (x - \mu_i) \right]$$
$$g_i(x) = -\frac{1}{2} (x - \mu_i)^T \Sigma_i^{-1} (x - \mu_i) - \frac{d}{2} \ln 2\pi - \frac{1}{2} \ln |\Sigma_i| + \ln P(\omega_i)$$

$$P(\text{error}) = \int_{R_2} p(x|\omega_1) P(\omega_1) dx + \int_{R_1} p(x|\omega_2) P(\omega_2) dx$$
$$P(\text{correct}) = \sum_{i=1}^c P(x \in \mathcal{R}_i, \omega_i)$$
$$= \sum_{i=1}^c P(x \in \mathcal{R}_i | \omega_i) P(\omega_i)$$
$$= \sum_{i=1}^c \int_{\mathcal{R}_i} p(x|\omega_i) P(\omega_i) dx$$

Naïve Bayes Classifier

- Given $x = (x_1, \dots, x_p)^T$
 - Goal is to predict class ω
 - Specifically, we want to find the value of ω that maximizes $P(\omega|x) = P(\omega|x_1, \dots, x_p)$
$$P(\omega|x_1, \dots, x_p) \propto P(x_1, \dots, x_p|\omega) P(\omega)$$
- Independence assumption among features
$$P(x_1, \dots, x_p|\omega) = P(x_1|\omega) \dots P(x_p|\omega)$$

How to Estimate Probabilities from Data?

Tid	Refund	Marital Status	Taxable Income	Evade
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

- Class: $P(\omega_k) = \frac{N_{\omega_k}}{N}$
 - e.g., $P(\text{No}) = 7/10$, $P(\text{Yes}) = 3/10$
- For discrete attributes:
$$P(x_i|\omega_k) = \frac{|x_{ik}|}{N_{\omega_k}}$$
 - where $|x_{ik}|$ is number of instances having attribute x_i and belongs to class ω_k
 - Examples:
$$P(\text{Status}=\text{Married}|\text{No}) = 4/7$$
$$P(\text{Refund}=\text{Yes}|\text{Yes}) = 0$$