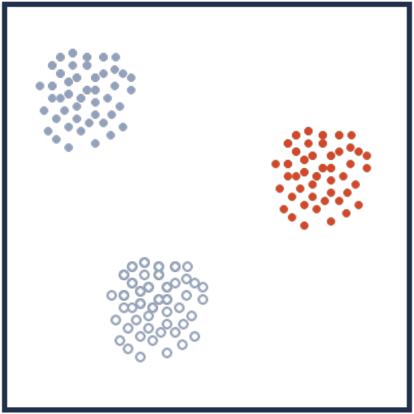
Unsupervised Learning

Creating our own truth



Clustering

Evaluation Metrics

- Withholding ground truth
- Unknown ground truth

Withholding Ground Truth

Problem Definition

We define a problem having k clusters and n samples with k pre-determined classes. C is the grouping of samples based on their classes and P is the grouping based on their predicted clusters.

Contingency Matrix

$X \backslash Y$	Y_1	Y_2	$\dots$	Y_s	Sums
X_1	n_{11}	n_{12}	$\dots$	n_{1s}	a_1
X_2	n_{21}	n_{22}	$\dots$	n_{2s}	a_2
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
X_r	n_{r1}	n_{r2}	$\dots$	n_{rs}	a_r
Sums	b_1	b_2	$\dots$	b_s	

Adjusted Rand Index

$$rand = \frac{w + d}{\binom{n}{2}},$$

where w is the number of pairs that are within the same group in both C and P, and d is the number of pairs that are in different groups in both C and P.

Adjusted Rand Index

$$\text{ARI} = \frac{\sum_{ij} \binom{n_{ij}}{2} + \left[\sum_i \binom{a_i}{2} \sum_j \binom{b_j}{2}\right] / \binom{n}{2}}{\left[\sum_i \binom{a_i}{2} + \sum_j \binom{b_j}{2}\right] / 2 - \left[\sum_i \binom{a_i}{2} \sum_j \binom{b_j}{2}\right] / \binom{n}{2}}.$$

Adjusted Rand Index

$$\begin{aligned}
\text{ARI} &= \frac{\sum_{ij}\binom{n_{ij}}{2} + \left[\sum_i \binom{a_i}{2} \sum_j \binom{b_j}{2}\right] / \binom{n}{2}}{\left[\sum_i \binom{a_i}{2} + \sum_j \binom{b_j}{2}\right]/2 - \left[\sum_i \binom{a_i}{2} \sum_j \binom{b_j}{2}\right] / \binom{n}{2}} \\
&= \frac{\text{Index} + \text{Expected Index}}{\text{Max Index} - \text{Expected Index}}.
\end{aligned}$$

Adjusted Mutual Information - Entropy

$$H(U) = -\sum_{i=1}^{|U|} P_U(i) \log(P_U(i)).$$

Adjusted Mutual Information - MI

$$MI(U,V) = \sum_{i=1}^{|U|} \sum_{j=1}^{|V|} P_{U,V}(i,j) \log\left(\frac{P_{U,V}(i,j)}{P_U(i)P_V(j)}\right).$$

Adjusted Mutual Information - NMI

$$NMI(U, V) = \frac{MI(U, V)}{\sqrt{H(U)H(V)}}.$$

Adjusted Mutual Information

$$\text{AMI} = \frac{\text{MI} - \text{Expected MI}}{\text{Max Entropy of U or V} - \text{Expected MI}}.$$

Homogeneity, Completeness, V-Measure - Entropy

$$H(C) = -\sum_{i=1}^{|C|} \frac{n_i}{n} \log(\frac{n_i}{n}).$$

Homogeneity, Completeness, V-Measure - Conditional Entropy

$$H(C \mid P) = -\sum_{i=1}^{|C|} \sum_{j=1}^{|P|} \frac{n_{i,j}}{n} \log(\frac{n_{i,j}}{n_j}).$$

Homogeneity, Completeness, V-Measure

$$\text{Homogeneity} = 1 - \frac{H(C \mid P)}{H(C)}$$

$$\text{Completeness} = 1 - \frac{H(P \mid C)}{H(P)}$$

$$\text{V-Measure} = \frac{2 \times \text{Homogeneity} \times \text{Completeness}}{\text{Homogeneity} + \text{Completeness}}$$

Unknown Ground Truth

Silhouette

$$\hat{w}_{i,k} = ||x_i - \hat{x}_k||_p^r, \hat{d}_{i,k} = ||x_i - \hat{x}_l||_p^r,$$

where $\hat{x}_k$ is the mean of all the points in cluster k

Silhouette

$$\text{Silhouette}_i = \frac{\hat{d}_{i,k} - \hat{w}_{i,k}}{\max(\hat{w}_{i,k}, \hat{d}_{i,k})}$$

Methods

$$\min_{\mu} \sum_{i=1}^{k} \sum_{x_j \in C_i} ||x_j - \mu_i||_2^2,$$

where μ_i is the centroid of cluster i and C_i is the subset of points that belong to cluster i.

K Means

Algorithm 1: K Means Solution Algorithm

Input: Features from data

Output: Centroids of the k clusters

Initialize cluster centroids (randomly or using a particular strategy)

while *cluster centroids update not converge* **do**

  Determine cluster for each point based on distance to centroids

  Update centroids' location as the mean of points in the cluster

Simple Demo

Involved Demo

Questions