Clustering Validation: Basic Concepts

Clustering Validation and Assessment

- Major issues on clustering validation and assessment
  - **Clustering evaluation**
    - Evaluating the goodness of the clustering
  - **Clustering stability**
    - To understand the sensitivity of the clustering result to various algorithm parameters, e.g., # of clusters
  - **Clustering tendency**
    - Assess the suitability of clustering, i.e., whether the data has any inherent grouping structure

Clustering Evaluation: Measuring Clustering Quality

Measuring Clustering Quality

- **Clustering Evaluation**: Evaluating the goodness of clustering results
  - No commonly recognized best suitable measure in practice
- **Three categorization of measures**: External, internal, and relative
  - **External**: Supervised, employ criteria not inherent to the dataset
    - Compare a clustering against prior or expert-specified knowledge (i.e., the ground truth) using certain clustering quality measure
  - **Internal**: Unsupervised, criteria derived from data itself
    - Evaluate the goodness of a clustering by considering how well the clusters are separated and how compact the clusters are, e.g., silhouette coefficient
  - **Relative**: Directly compare different clusterings, usually those obtained via different parameter settings for the same algorithm

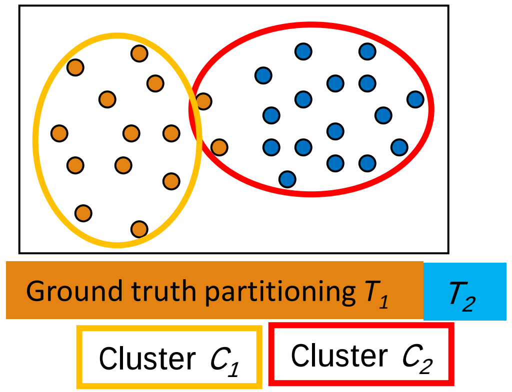
External Measures for Clustering Validation

Measuring Clustering Quality: External Methods

- Given the **ground truth** T, $Q(C, T)$ is the **quality measure** for a clustering C
- $Q(C, T)$ is good if it satisfies the following **four** essential criteria
  - **Cluster homogeneity**
    - The purer, the better
  - **Cluster completeness**
    - Assign objects belonging to the same category in the ground truth to the same cluster
  - **Rag bag better than alien**
    - Putting a heterogeneous object into a pure cluster should be penalized more than putting it into a *rag bag* (i.e., “miscellaneous” or “other” category)
  - **Small cluster preservation**
    - Splitting a small category into pieces is more harmful than splitting a large category into pieces

Commonly Used External Measures

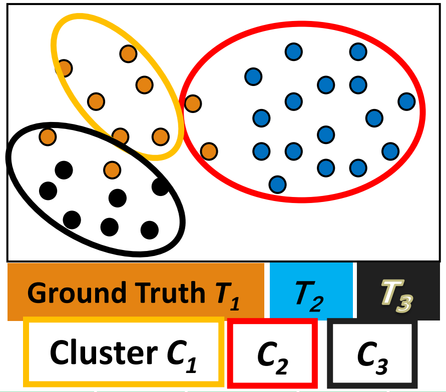
- **Matching-based measures** (To be covered)
  - Purity, maximum matching, F-measure
- **Entropy-Based Measures**
  - Conditional entropy (To be covered)
  - Normalized mutual information (NMI) (To be covered)
  - Variation of information
- **Pairwise measures** (To be covered)
  - Four possibilities: True positive (TP), FN, FP, TN
  - Jaccard coefficient, Rand statistic, Fowlkes-Mallow measure
- **Correlation measures**
  - Discretized Huber static, normalized discretized Huber static



External Measures I: Matching-Based Measures

Matching-Based Measures (I): Purity vs. Maximum Matching

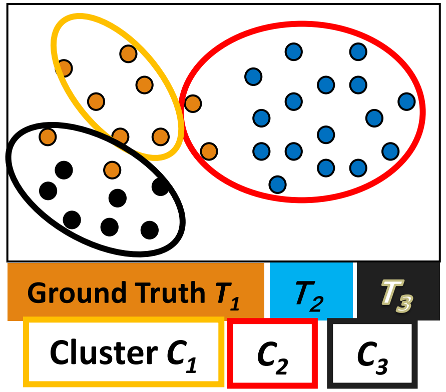
- **Purity**: Quantifies the extent that cluster C_i contains points only from one (ground truth) partition: $purity_i = \frac{1}{n_i} \max_{j=1}^{k} \{n_{ij}\}$
  - Total purity of clustering C: $$purity = \sum_{i=1}^{r} \frac{n_i}{n} purity_i = \frac{1}{n} \sum_{i=1}^{r} \max_{j=1}^{k} \{n_{ij}\}$$
  - Perfect clustering if purity = 1 and $r = k$ (the number of clusters obtained is the same as that in the ground truth)
  - Ex. 1 (green or orange): $purity_1 = 30/50$; $purity_2 = 20/25$; $purity_3 = 25/25$; $purity = (30 + 20 + 25)/100 = 0.75$
  - Two clusters may share the same majority partition
- **Maximum matching**: Only one cluster can match one partition
  - Match: Pairwise matching, weight $w(e_{ij}) = n_{ij}$ $\quad \mathrm{w(M)} = \sum_{e \in M} w(e)$
  - Maximum weight matching: $match = \arg\max_{M} \{\frac{w(M)}{n}\}$
  - Ex2. (green) $match = purity =$ 0.75; (orange) $match$ = 0.65 > 0.6



C\T	T_1	T_2	T_3	Sum
C_1	0	20	30	50
C_2	0	20	5	25
C_3	25	0	0	25
m_j	25	40	35	100

C\T	T_1	T_2	T_3	Sum
C_1	0	30	20	50
C_2	0	20	5	25
C_3	25	0	0	25
m_j	25	50	25	100

Matching-Based Measures (II): F-Measure



- **Precision**: The fraction of points in C_i from the majority partition T_{j_i} (i.e., the same as purity), where j_i is the partition that contains the maximum # of points from C_i

$$prec_i = \frac{1}{n_i}\max_{j=1}^{k}\{n_{ij}\} = \frac{n_{ij_i}}{n_i}$$

  - Ex. For the green table
    - $prec_1$ = 30/50; $prec_2$ = 20/25; $prec_3$ = 25/25

C\T	T_1	T_2	T_3	Sum
C_1	0	20	30	50
C_2	0	20	5	25
C_3	25	0	0	25
m_j	25	40	35	100

- **Recall**: The fraction of point in partition T_{j_i} shared in common with cluster C_i, where $m_{j_i} = |T_{j_i}|$

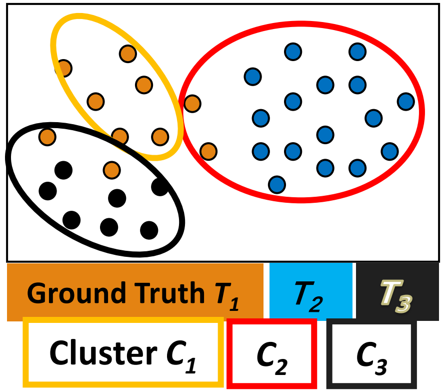
$$recall_i = \frac{n_{ij_i}}{|T_{j_i}|} = \frac{n_{ij_i}}{m_{j_i}}$$

  - Ex. For the green table
    - $recall_1$ = 30/35; $recall_2$ = 20/40; $recall_3$ = 25/25
- **F-measure** for C_i: The harmonic means of $prec_i$ and $recall_i$: $F_i = \frac{2n_{ij_i}}{n_i + m_{j_i}}$
- F-measure for clustering C: average of all clusters: $F = \frac{1}{r}\sum_{i=1}^{r} F_i$
  - Ex. For the green table
    - F_1 = 60/85; F_2 = 40/65; F_3 = 1; F = 0.774

External Measures II: Entropy-Based Measures

Entropy-Based Measures (I): Conditional Entropy

- **Entropy of clustering** $\mathcal{C}$: $H(\mathcal{C}) = -\sum_{i=1}^{r} p_{C_i} \log p_{C_i}$ $\quad p_{C_i} = \frac{n_i}{n}$ (i.e., the probability of cluster C_i)
- **Entropy of partitioning** $\mathcal{T}$: $H(\mathcal{T}) = -\sum_{j=1}^{k} p_{T_j} \log p_{T_j}$
- **Entropy of** $\mathcal{T}$ **with respect to cluster** C_i: $H(\mathcal{T}|C_i) = -\sum_{j=1}^{k} (\frac{n_{ij}}{n_i}) \log(\frac{n_{ij}}{n_i})$
- **Conditional entropy of** $\mathcal{T}$ **with respect to clustering** $\mathcal{C}$: $H(\mathcal{T}|\mathcal{C}) = -\sum_{i=1}^{r} (\frac{n_i}{n}) H(\mathcal{T}|C_i) = -\sum_{i=1}^{r} \sum_{j=1}^{k} p_{ij} \log(\frac{p_{ij}}{p_{C_i}})$
  - The more a cluster's members are split into different partitions, the higher the conditional entropy
  - For a perfect clustering, the conditional entropy value is 0, where the worst possible conditional entropy value is *log k*

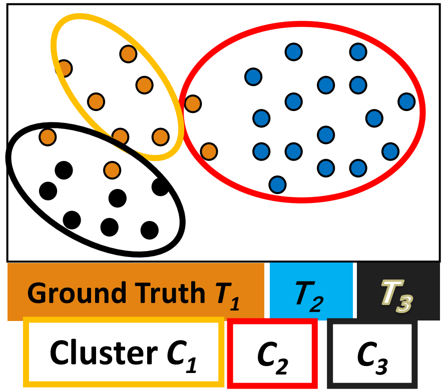


$$H(\mathcal{T}|\mathcal{C}) = -\sum_{i=1}^{r} \sum_{j=1}^{k} p_{ij} (\log p_{ij} - \log p_{C_i}) = -\sum_{i=1}^{r} \sum_{j=1}^{k} p_{ij} \log p_{ij} + \sum_{i=1}^{r} (\log p_{C_i} \sum_{j=1}^{k} p_{ij})$$

$$= -\sum_{i=1}^{r} \sum_{j=1}^{k} p_{ij} \log p_{ij} + \sum_{i=1}^{r} (p_{C_i} \log p_{C_i}) = H(\mathcal{C}, \mathcal{T}) - H(\mathcal{C})$$

Entropy-Based Measures (II): Normalized Mutual Information (NMI)

- **Mutual information**:
  - Quantifies the amount of shared info between the clustering C and partitioning T
    $$I(C,T) = \sum_{i=1}^{r}\sum_{j=1}^{k} p_{ij} \log\left(\frac{p_{ij}}{p_{C_i} \cdot p_{T_j}}\right)$$
  - Measures the dependency between the observed joint probability p_{ij} of C and T, and the expected joint probability $p_{Ci} \cdot p_{Tj}$ under the independence assumption
  - When C and T are independent, $p_{ij} = p_{Ci} \cdot p_{Tj}$, $I(C, T) = 0$. However, there is no upper bound on the mutual information



- **Normalized mutual information** (NMI)

$$NMI(C,T) = \sqrt{\frac{I(C,T)}{H(C)} \cdot \frac{I(C,T)}{H(T)}} = \frac{I(C,T)}{\sqrt{H(C) \cdot H(T)}}$$

  - Value range of NMI: [0,1]. Value close to 1 indicates a good clustering

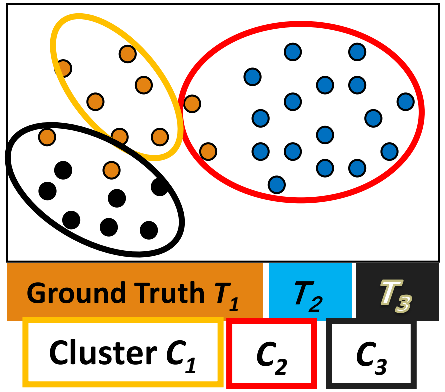
External Measures III: Pairwise Measures

Pairwise Measures: Four Possibilities for Truth Assignment

- **Four possibilities** based on the agreement between cluster label and partition label
  - *TP*: true positive—Two points $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ belong to the same partition *T*, and they also in the same cluster *C*

$$TP = |\{(\mathbf{x}_i, \mathbf{x}_j) : y_i = y_j \text{ and } \hat{y}_i = \hat{y}_j\}|$$

where y_i: the true partition label , and $\hat{y}_i$: the cluster label for point $\boldsymbol{x}_i$



  - *FN*: false negative: $FN = |\{(\mathbf{x}_i, \mathbf{x}_j) : y_i = y_j \text{ and } \hat{y}_i \neq \hat{y}_j\}|$
  - *FP: false positive* $FP = |\{(\mathbf{x}_i, \mathbf{x}_j) : y_i \neq y_j \text{ and } \hat{y}_i = \hat{y}_j\}|$
  - *TN*: true negative $TN = |\{(\mathbf{x}_i, \mathbf{x}_j) : y_i \neq y_j \text{ and } \hat{y}_i \neq \hat{y}_j\}|$
- Calculate the four measures:

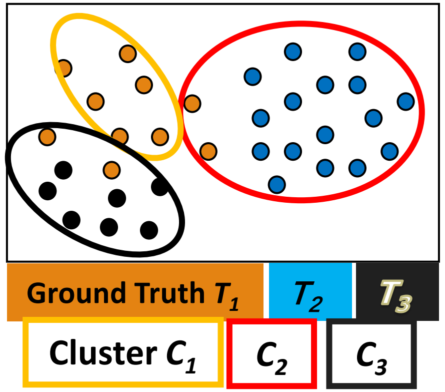
$$N = \binom{n}{2}$$

Total # of pairs of points

$$TP = \sum_{i=1}^{r}\sum_{j=1}^{k}\binom{n_{ij}}{2} = \frac{1}{2}\left(\left(\sum_{i=1}^{r}\sum_{j=1}^{k} n_{ij}^{\;2}\right) - n\right) \quad FN = \sum_{j=1}^{k}\binom{m_j}{2} - TP$$

$$FP = \sum_{i=1}^{r}\binom{n_i}{2} - TP \quad TN = N - (TP + FN + FP) = \frac{1}{2}\left(n^2 - \sum_{i=1}^{r} n_i^{\;2} - \sum_{j=1}^{k} m_j^{\;2} + \sum_{i=1}^{r}\sum_{j=1}^{k} n_{ij}^{\;2}\right)$$

Pairwise Measures: Jaccard Coefficient and Rand Statistic



- **Jaccard coefficient:** Fraction of true positive point pairs, but after ignoring the true negatives (thus asymmetric)
  - $Jaccard = TP/(TP + FN + FP)$ [i.e., denominator ignores TN]
  - Perfect clustering: $Jaccard = 1$
- **Rand Statistic**:
  - $Rand = (TP + TN)/N$
  - Symmetric; perfect clustering: $Rand = 1$
- **Fowlkes-Mallow Measure**:
  - Geometric mean of precision and recall

$$FM = \sqrt{prec \times recall} = \frac{TP}{\sqrt{(TP+FN)(TP+FP)}}$$

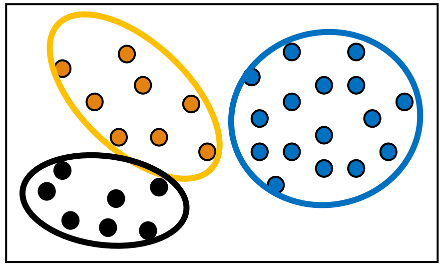
- Using the above formulas, one can calculate all the measures for the green table (leave as an exercise)

$C \backslash T$	T_1	T_2	T_3	Sum
C_1	0	20	30	50
C_2	0	20	5	25
C_3	25	0	0	25
m_j	25	40	35	100

Internal Measures for Clustering Validation

Internal Measures (I): BetaCV Measure

- A trade-off in maximizing intra-cluster compactness and inter-cluster separation
- Given a clustering $C = \{C_1, . . ., C_k\}$ with k clusters, cluster C_i containing $n_i = |C_i|$ points
  - Let $W(S, R)$ be sum of weights on all edges with one vertex in S and the other in R
  - The sum of all the intra-cluster weights over all clusters: $W_{in} = \frac{1}{2}\sum_{i=1}^{k} W(C_i, C_i)$
  - The sum of all the inter-cluster weights: $W_{out} = \frac{1}{2}\sum_{i=1}^{k} W(C_i, \overline{C_i}) = \sum_{i=1}^{k-1}\sum_{j>i} W(C_i, C_j)$
  - The number of distinct intra-cluster edges: $N_{in} = \sum_{i=1}^{k} \binom{n_i}{2}$
  - The number of distinct inter-cluster edges: $N_{out} = \sum_{i=1}^{k-1}\sum_{j=i+1}^{k} n_i n_j$



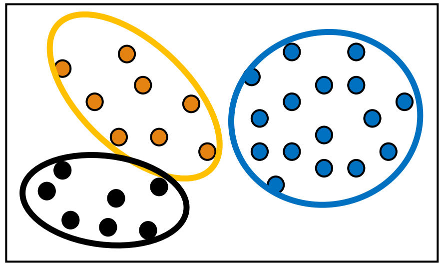
- **Beta-CV measure**: $BetaCV = \frac{W_{in} / N_{in}}{W_{out} / N_{out}}$
  - The ratio of the mean intra-cluster distance to the mean inter-cluster distance
  - The smaller, the better the clustering

Internal Measures (II): Normalized Cut and Modularity

- **Normalized cut**: $$NC = \sum_{i=1}^{k} \frac{W(C_i, \overline{C_i})}{vol(C_i)} = \sum_{i=1}^{k} \frac{W(C_i, \overline{C_i})}{W(C_i, \mathrm{V})} = \sum_{i=1}^{k} \frac{W(C_i, \overline{C_i})}{W(C_i, C_i) + W(C_i, \overline{C_i})} = \sum_{i=1}^{k} \frac{1}{\frac{W(C_i, C_i)}{W(C_i, \overline{C_i})} + 1}$$

  where $vol(C_i) = W(C_i, V)$ is the volume of cluster C_i

  - The higher normalized cut value, the better the clustering

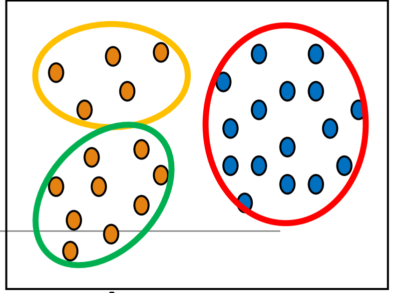


- **Modularity** (for graph clustering) $$Q = \sum_{i=1}^{k} \left(\frac{W(C_i, C_i)}{W(V,V)} - \left(\frac{W(C_i, V)}{W(V,V)} \right)^2 \right)$$
  - Modularity Q is defined as

    where $$W(V,V) = \sum_{i=1}^{k} W(C_i, V) = \sum_{i=1}^{k} W(C_i, C_i) + \sum_{i=1}^{k} W(C_i, \overline{C_i}) = 2(W_{in} + W_{out})$$
  - Modularity measures the difference between the observed and expected fraction of weights on edges within the clusters.
  - The smaller the value, the better the clustering—the intra-cluster distances are lower than expected

Relative Measures

Relative Measure



- Relative measure: Directly compare different clusterings, usually those obtained via different parameter settings for the same algorithm
- **Silhouette coefficient** as an **internal measure**: Check cluster cohesion and separation
  - For each point $\boldsymbol{x}_i$, its silhouette coefficient s_i is: $s_i = \frac{\mu_{out}^{\min}(\mathbf{x}_i) - \mu_{in}(\mathbf{x}_i)}{\max\{\mu_{out}^{\min}(\mathbf{x}_i), \mu_{in}(\mathbf{x}_i)\}}$

    where $\mu_{in}(\mathbf{x}_i)$ is the mean distance from $\boldsymbol{x}_i$ to points in its own cluster

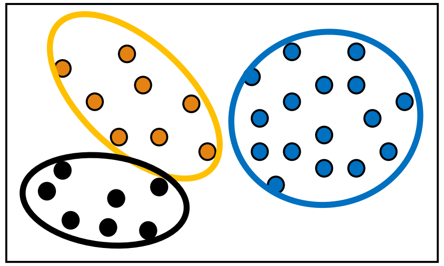
    $\mu_{out}^{\min}(\mathbf{x}_i)$ is the mean distance from $\boldsymbol{x}_i$ to points in its closest cluster
  - Silhouette coefficient (*SC*) is the mean values of s_i across all the points: $SC = \frac{1}{n}\sum_{i=1}^{n} s_i$
  - *SC* close to +1 implies good clustering
    - Points are close to their own clusters but far from other clusters
- **Silhouette coefficient** as a **relative measure**: Estimate the # of clusters in the data

$$SC_i = \frac{1}{n_i}\sum_{x_j \in C_i} s_j$$

Pick the k value that yields the best clustering, i.e., yielding high values for *SC* and SC_i ($1 \le i \le k$)

Cluster Stability

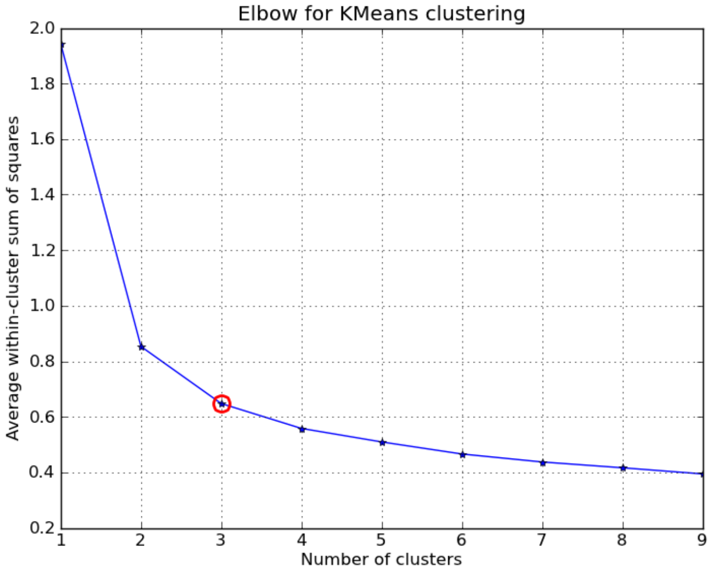
Cluster Stability



- Clusterings obtained from several datasets sampled from the same underlying distribution as ***D*** should be similar or "stable"
- Typical approach:
  - Find good parameter values for a given clustering algorithm
- Example: Find a good value of k, the correct number of clusters
- A **bootstrapping approach** to find the best value of k (judged on stability)
  - Generate t samples of size n by sampling from ***D*** with replacement
  - For each sample $\boldsymbol{D}_i$, run the same clustering algorithm with k values from 2 to k_{max}
  - Compare the distance between all pairs of clusterings $C_k(\boldsymbol{D}_i)$ and $C_k(\boldsymbol{D}_j)$ via some distance function
    - Compute the expected pairwise distance for each value of k
  - The value k^* that exhibits the least deviation between the clusterings obtained from the resampled datasets is the best choice for k since it exhibits the most stability

Other Methods for Finding K, the Number of Clusters

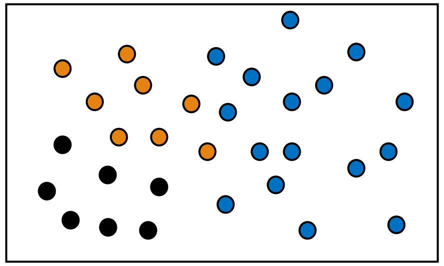
- **Empirical method**
  - # of clusters: $k \approx \sqrt{n/2}$ for a dataset of n points (e.g., n = 200, k = 10)
- **Elbow method**: Use the turning point in the curve of the sum of within cluster variance with respect to the # of clusters



- **Cross validation method**
  - Divide a given data set into m parts
  - Use $m - 1$ parts to obtain a clustering model
  - Use the remaining part to test the quality of the clustering
    - For example, for each point in the test set, find the closest centroid, and use the sum of squared distance between all points in the test set and the closest centroids to measure how well the model fits the test set
  - For any $k > 0$, repeat it m times, compare the overall quality measure w.r.t. different k's, and find # of clusters that fits the data the best

Clustering Tendency

Clustering Tendency: Whether the Data Contains Inherent Grouping Structure

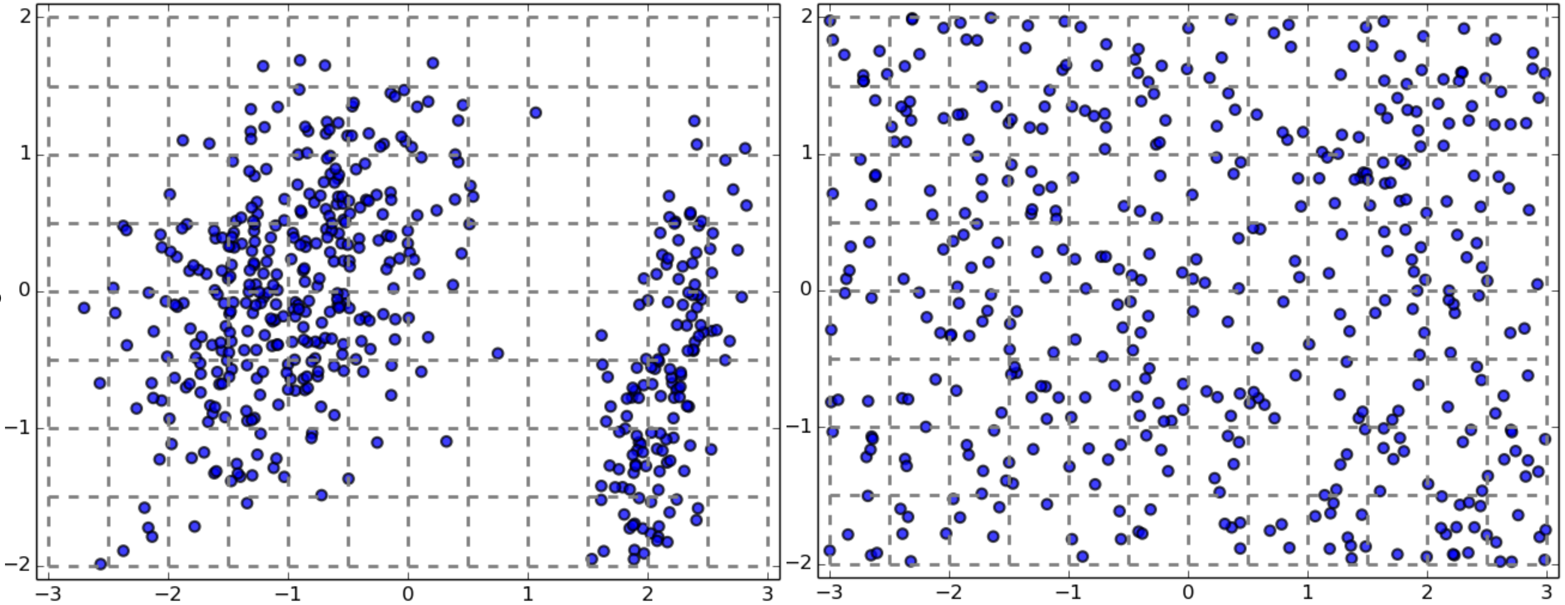


- Assessing the **suitability of clustering**
  - (i.e., whether the data has any inherent grouping structure)
- Determining ***clustering tendency*** or ***clusterability***
  - **A hard task** because there are so many different definitions of clusters
    - E.g., partitioning, hierarchical, density-based, graph-based, etc.
  - Even fixing cluster type, still hard to define an appropriate null model for a data set
- Still, there are some **clusterability assessment methods**, such as
  - **Spatial histogram**: Contrast the histogram of the data with that generated from random samples

    To be covered here
  - **Distance distribution**: Compare the pairwise point distance from the data with those from the randomly generated samples
  - **Hopkins Statistic**: A sparse sampling test for spatial randomness

Testing Clustering Tendency: A Spatial Histogram Approach

- **Spatial Histogram Approach:** Contrast the *d*-dimensional histogram of the input dataset ***D*** with the histogram generated from random samples
  - Dataset D is clusterable if the distributions of two histograms are rather different
- Method outline
  - Divide each dimension into equi-width bins, count how many points lie in each cells, and obtain the empirical joint probability mass function (EPMF)



  - Do the same for the randomly sampled data
  - Compute how much they differ using the *Kullback-Leibler* (*KL*) *divergence* value

Recommended Readings

- M. J. Zaki and W. Meira, Jr.. Data Mining and Analysis: Fundamental Concepts and Algorithms. Cambridge University Press, 2014
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