Clustering Evaluation

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These slides are inspired based on slides from Mohammed Zaki, Chao Zhang, and Jiawei Han.

Clustering Evaluation

- Clustering evaluation aims at quantifying the goodness or quality of the clustering.

- Two main categories of measures:
  - **External measures**: employ external ground-truth
  - **Internal measures**: derive goodness from the data itself

Outline

- External measures for clustering evaluation
  - Matching-based measures
  - Entropy-based measures
  - Pairwise measures
- Internal measures for clustering evaluation
  - Graph-based measures
  - Davies-Bouldin Index
  - Silhouette Coefficient

External Measures

External measures assume that the correct or ground-truth clustering is known *a priori*, which is used to evaluate a given clustering.

Let $\mathbf{D} = \{\mathbf{x}_i\}_{i=1}^{n}$ be a dataset consisting of n points in a d-dimensional space, partitioned into k clusters. Let $y_i \in \{1, 2, \ldots, k\}$ denote the ground-truth cluster membership or label information for each point.

The ground-truth clustering is given as $\mathcal{T} = \{T_1, T_2, \ldots, T_k\}$, where the cluster T_j consists of all the points with label j, i.e., $T_j = \{\mathbf{x}_i \in \mathbf{D} | y_i = j\}$. We refer to $\mathcal{T}$ as the ground-truth *partitioning*, and to each T_i as a *partition*.

Let $\mathcal{C} = \{C_1, \ldots, C_r\}$ denote a clustering of the same dataset into r clusters, obtained via some clustering algorithm, and let $\hat{y}_i \in \{1, 2, \ldots, r\}$ denote the cluster label for $\mathbf{x}_i$.

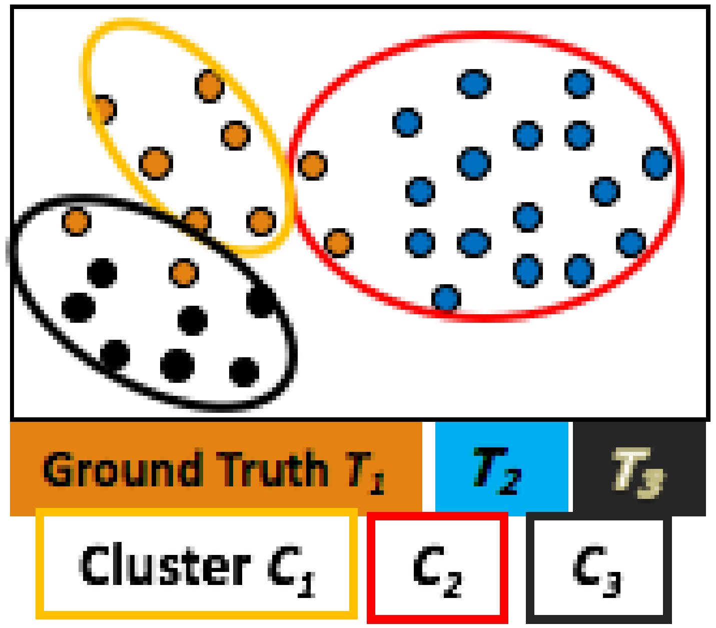
So **k** is the number of ground truth partitions (T) and **r** is the number of clusters (C) obtained by algorithm

n_{ij} = Number of data points in cluster **i** which are also in ground truth partition **j**

Matching-Based Measures (I): Purity

- **Purity**: Quantifies the extent that cluster C_i contains points only from one (ground truth) partition:

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



$$purity_3 = \frac{1}{n_3}\max(n_{31}, n_{32}, n_{33})$$

$$= \frac{1}{9}\max(2,0,7) = \frac{7}{9}$$

The Total purity of clustering C is the weighted sum of the cluster-wise purity:

$$purity = \sum_{i=1}^{r} \frac{n_i}{n} purity_i = \frac{1}{n} \sum_{i=1}^{r} \max_{j=1}^{k} \{n_{ij}\}$$

What is purity value for a perfect clustering? Purity = 1

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

$$purity = \sum_{i=1}^{r} \frac{n_i}{n} purity_i = \frac{1}{n} \sum_{i=1}^{r} \max_{j=1}^{k} \{n_{ij}\}$$

Example:

purity1 = 30/50;
purity2 = 20/25;
purity3 = 25/25;
purity = (30 + 20 + 25)/100 = 0.75

$C\backslash T$	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

Two clusters may be matched to the same partition

C1 is more paired with T3
C2 is more paired with T2

$C \backslash T$	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

purity = (30 + 20 + 25)/100 = 0.75

C1 is more paired with T2
C2 is more paired with T2

$C \backslash T$	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

purity = (30 + 20 + 25)/100 = 0.75

Maximum weight matching: Only one cluster can match one partition

Ex. If C1 is more paired with T2 **THEN** C2 and C3 cannot paired with T2

$C \backslash T$	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

MAX

C1 is more paired with T2 = $\frac{30+5+25}{100} = 0.6$

C1 is more paired with T3 = $\frac{20+20+25}{100} = 0.65$

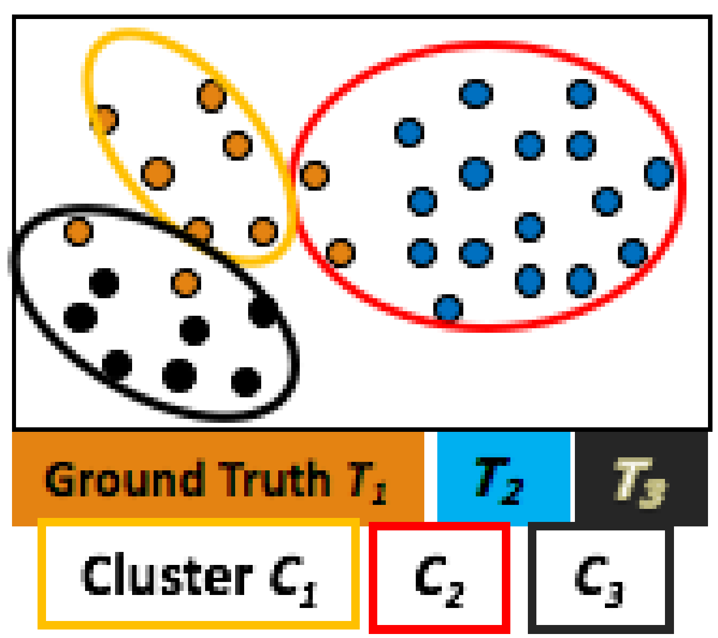
Purity = 0.65

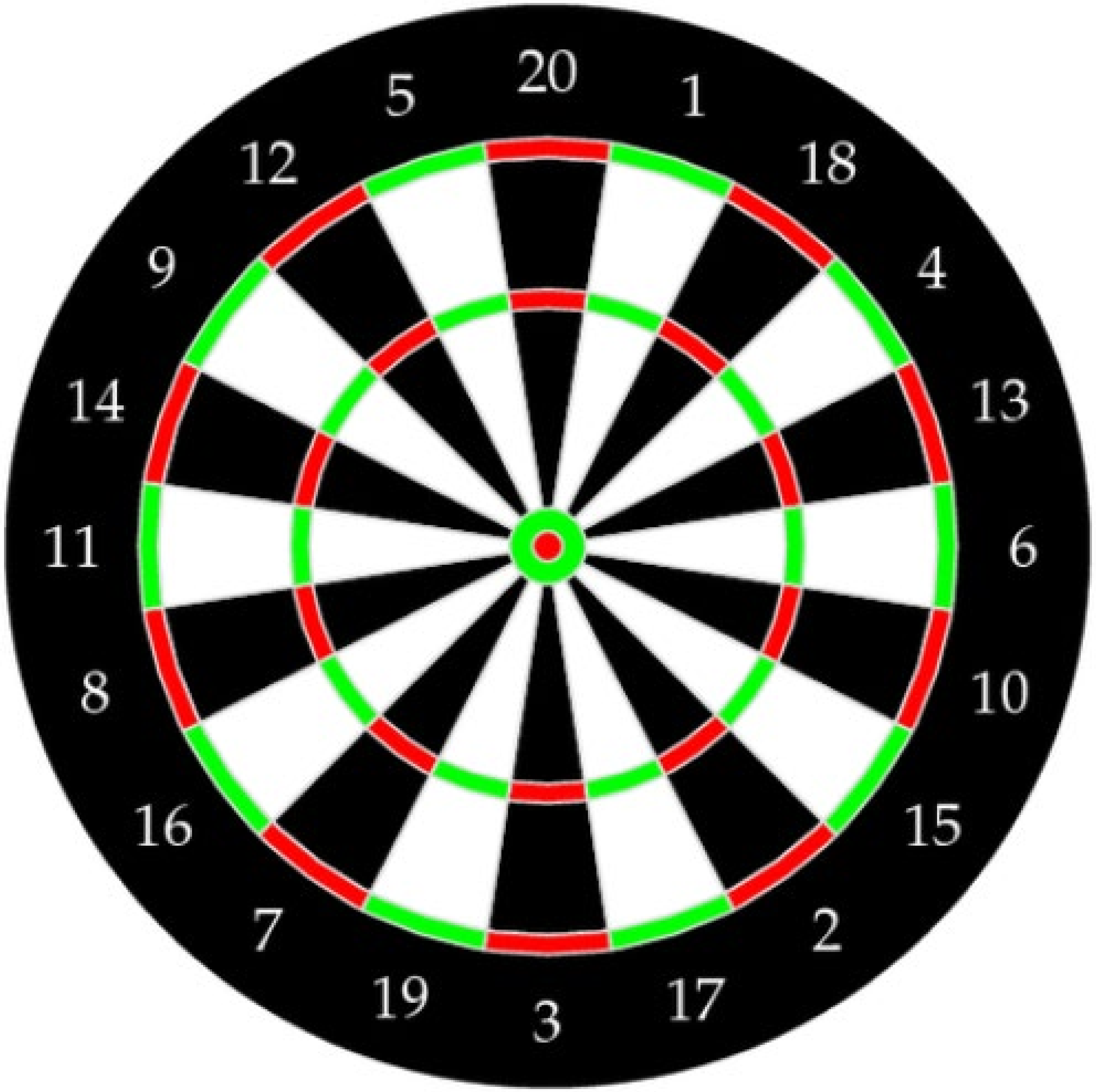
Matching-Based Measures (II): Maximum Matching

- **Drawback of purity**: two clusters may be matched to the same partition.
- **Maximum matching**: the maximum purity under the one-to-one matching constraint.
    - Examine all possible pairwise matching between C and T and choose the best (the maximum)

$C\backslash T$	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

Example:
Maximum matching = 0.65 > 0.6




20
1
18
4
13
6
10
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2
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3
19
7
16
8
11
14
9
12
5

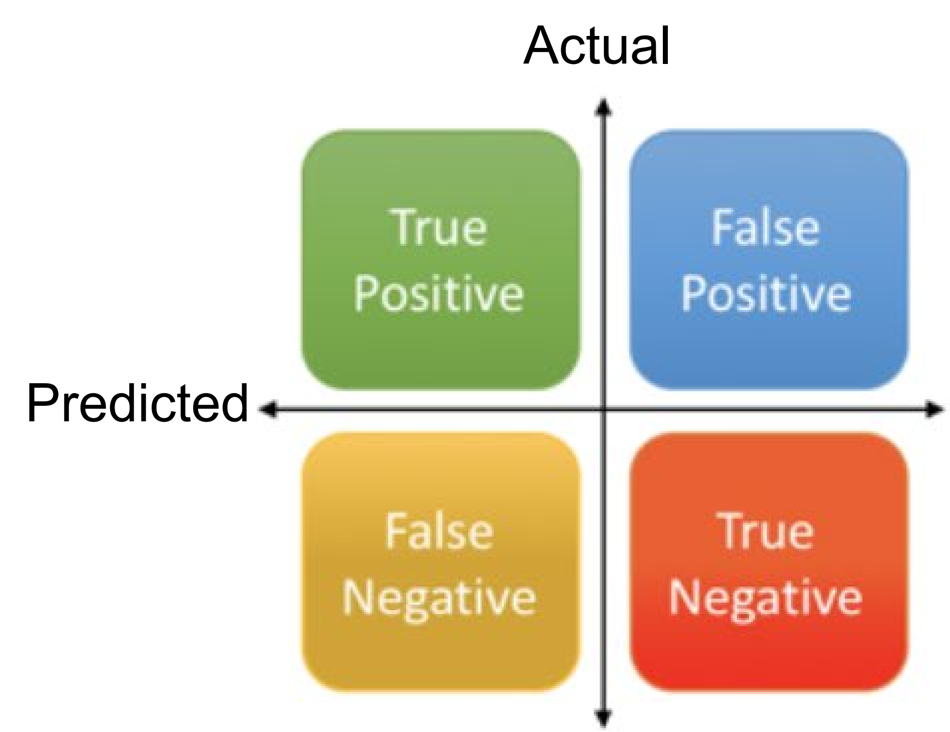
In a general context: **Precision, Recall and Accuracy**

	Correct prediction		Wrong prediction
Number of predicted "positive" labeled data =	True Positive	+	False Positive
Number of predicted "negative" labeled data =	True Negative	+	False Negative

$$\textbf{Precision} = \frac{\textit{True Positive}}{\textit{Predicted Results}} \text{ or } \frac{\text{True Positive}}{\text{True Positive + False Positive}}$$

$$\textbf{Recall} = \frac{\textit{True Positive}}{\textit{Actual Results}} \text{ or } \frac{\text{True Positive}}{\text{True Positive + False Negative}}$$

$$\textbf{Accuracy} = \frac{\text{True Positive + True Negative}}{\text{Total}}$$



False positive is also called false alarm

Matching-Based Measures (II): F-Measure

- **Precision**: which measure ***quality***, is the same as purity:
  - How precisely does each cluster represent the ground truth?

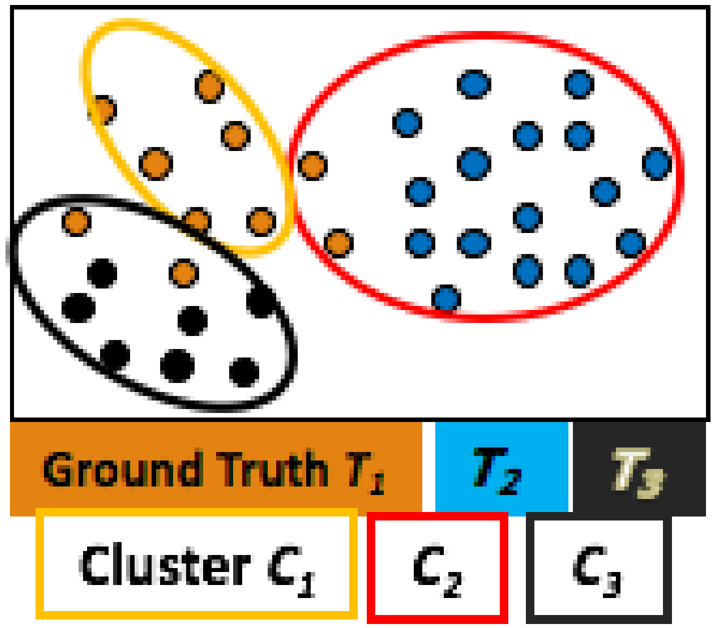
$$prec_i = \frac{1}{n_i} \max_{j=1}^{k} \{n_{ij}\} = \frac{n_{ij_i}}{n_i}$$

- **Recall**: measures completeness $recall_i = \frac{n_{ij_i}}{|T_{j_i}|} = \frac{n_{ij_i}}{m_{j_i}}$
  - How completely does each cluster recover the ground truth?

The Fraction of point in partition T_j shred in common with cluster C_i

$$Prec_1 = \frac{6}{6}$$

$$Recall_1 = \frac{6}{10}$$



Precision and Recall

(Precision here is same as the purity)

Precision:
$prec_1 = 30/50$;
$prec_2 = 20/25$;
$prec_3 = 25/25$

Recall:
$recall_1 = 30/35$;
$recall_2 = 20/40$;
$recall_3 = 25/25$

$C \backslash T$	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

Matching-Based Measures (II): F-Measure

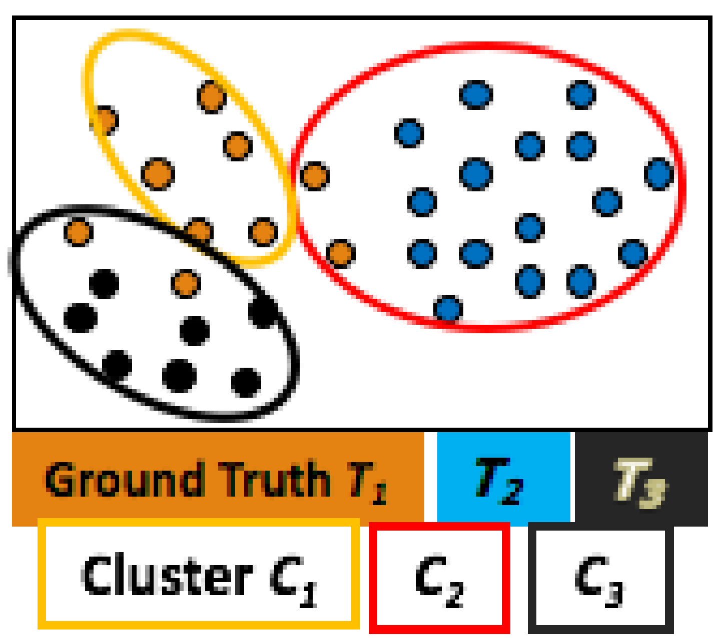
- **F-Measure**: the harmonic mean of precision and recall
  - Take into account both *precision* and *completeness*

$$F_i = \frac{2}{\frac{1}{prec_i} + \frac{1}{recall_i}} = \frac{2 \cdot prec_i \cdot recall_i}{prec_i + recall_i} = \frac{2\, n_{ij_i}}{n_i + m_{j_i}}$$

The F-measure for the clustering $\mathcal{C}$ is the mean of clusterwise F-measure values:

$$F = \frac{1}{r} \sum_{i=1}^{r} F_i$$

F1 = 60/85;
F2 = 40/65;
F3 = 1;
F = 0.774



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

Entropy-Based Measures (I): Conditional Entropy

Amount of information orderness in different partitions

- The entropy for clustering C and partition T is

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

where $p_{C_i} = \frac{n_i}{n}$ and $p_{T_j} = \frac{m_j}{n}$

i.e., The probability of cluster C_i
$n_i = n_{i1} + n_{i2} + \cdots + n_{ik}$

i.e., The probability of ground truth T_j

- **Conditional Entropy**: The cluster-specific entropy, namely the conditional entropy of T with respect to cluster C_i:

$$H(\mathcal{T}|C_i) = -\sum_{j=1}^{k} \left(\frac{n_{ij}}{n_i}\right) \log \left(\frac{n_{ij}}{n_i}\right)$$

How ground truth is distributed within each cluster

n_{ij}

Ground truth (T)

Cluster (C)

Entropy-Based Measures (I): Conditional Entropy

- The conditional entropy of T given clustering C is defined as the weighted sum:

$$\frac{n_{ij}}{n}$$

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

$$= H(\mathcal{C},\mathcal{T}) - H(\mathcal{C})$$

$$\frac{n_i}{n}$$

The more clusters members are split into different partitions, the higher the conditional entropy (not a desirable condition and the max value is log k)

$H(\mathcal{T}|\mathcal{C}) = 0$ if and only if $\mathcal{T}$ is completely determined by $\mathcal{C}$, corresponding to the ideal clustering. If $\mathcal{C}$ and $\mathcal{T}$ are independent of each other, then $H(\mathcal{T}|\mathcal{C}) = H(\mathcal{T})$.

$$H(Y|X) = \sum_{x \in X} p(x) H(Y|X = x)$$

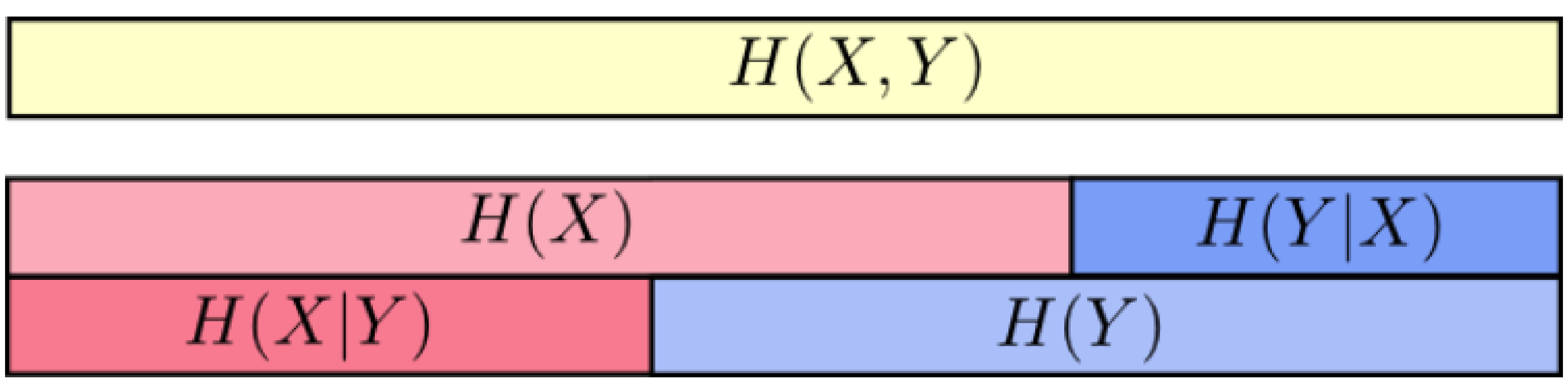
Fresh your memory:

$$H(Y|X) = H(X,Y) - H(X)$$

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

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

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



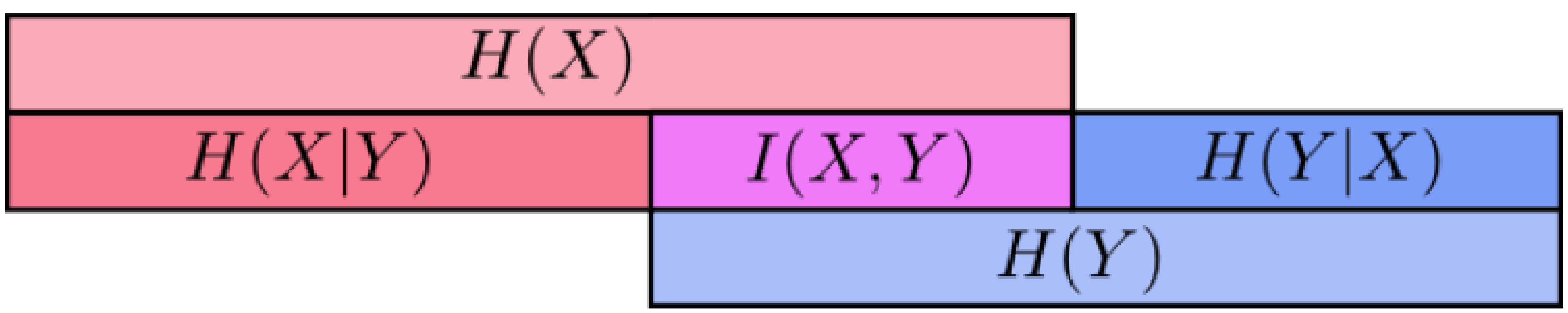
Entropy-Based Measures (I): Mutual Information

The *mutual information* tries to quantify the amount of shared information between the clustering $\mathcal{C}$ and partitioning $\mathcal{T}$, and it is defined as

$$I(\mathcal{C}, \mathcal{T}) = \sum_{i=1}^{r} \sum_{j=1}^{k} p_{ij} \log \left(\frac{p_{ij}}{p_{C_i} \cdot p_{T_j}} \right) = H(\mathcal{T}) - H(\mathcal{T}|\mathcal{C})$$

When $\mathcal{C}$ and $\mathcal{T}$ are independent then $p_{ij} = p_{C_i} \cdot p_{T_j}$, and thus $I(\mathcal{C}, \mathcal{T}) = 0$. However, there is no upper bound on the mutual information.

We should do something about this



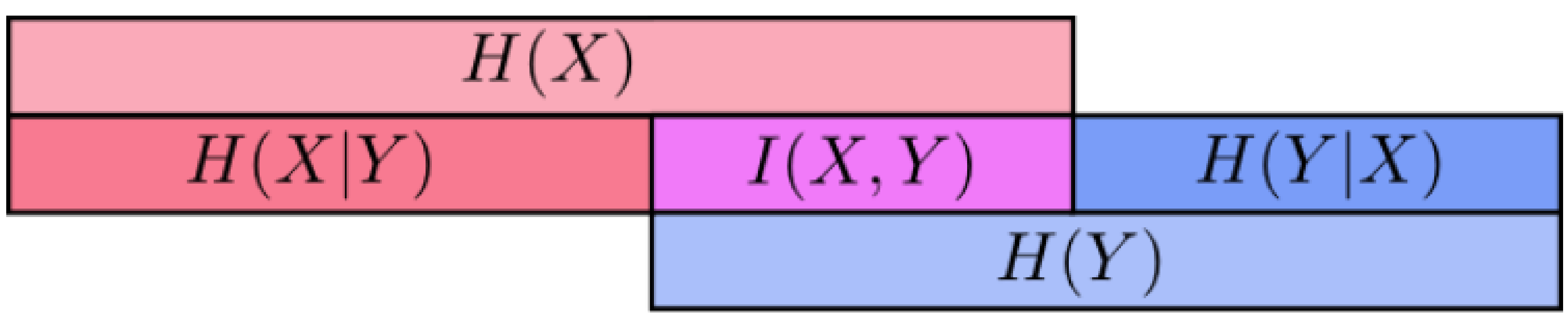
We measure the dependency between the observed joint probability p_{ij} of C and T, and the expected joint probability $p_{ci}.p_{Tj}$ under the independence assumption

Entropy-Based Measures (I): Mutual Information

The *normalized mutual information* (NMI) is defined as the geometric mean:

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

The NMI value lies in the range $[0,1]$. Values close to 1 indicate a good clustering.



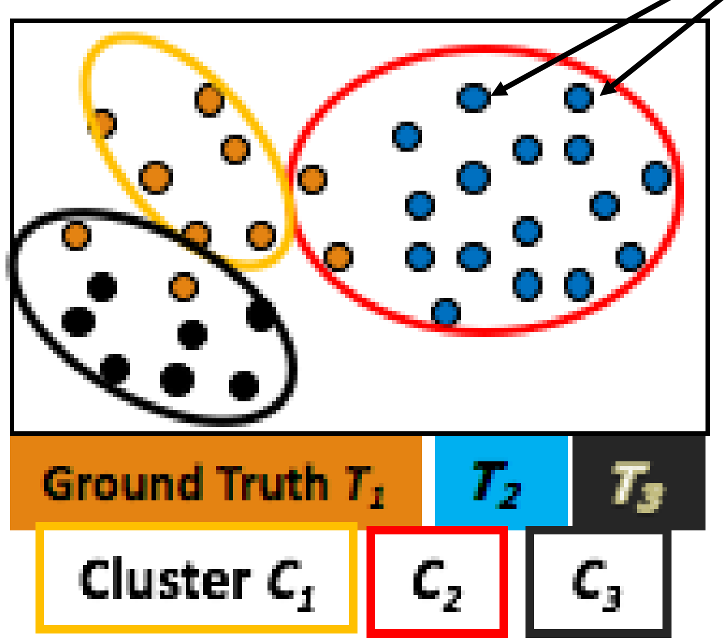
Pairwise Measures

Given clustering $\mathcal{C}$ and ground-truth partitioning $\mathcal{T}$, let $\mathbf{x}_i, \mathbf{x}_j \in \mathbf{D}$ be any two points, with $i \neq j$. Let y_i denote the true partition label and let $\hat{y}_i$ denote the cluster label for point $\mathbf{x}_i$.

True Positives: $\mathbf{x}_i$ and $\mathbf{x}_j$ belong to the same partition in $\mathcal{T}$, and they are also in the same cluster in $\mathcal{C}$. The number of true positive pairs is given as

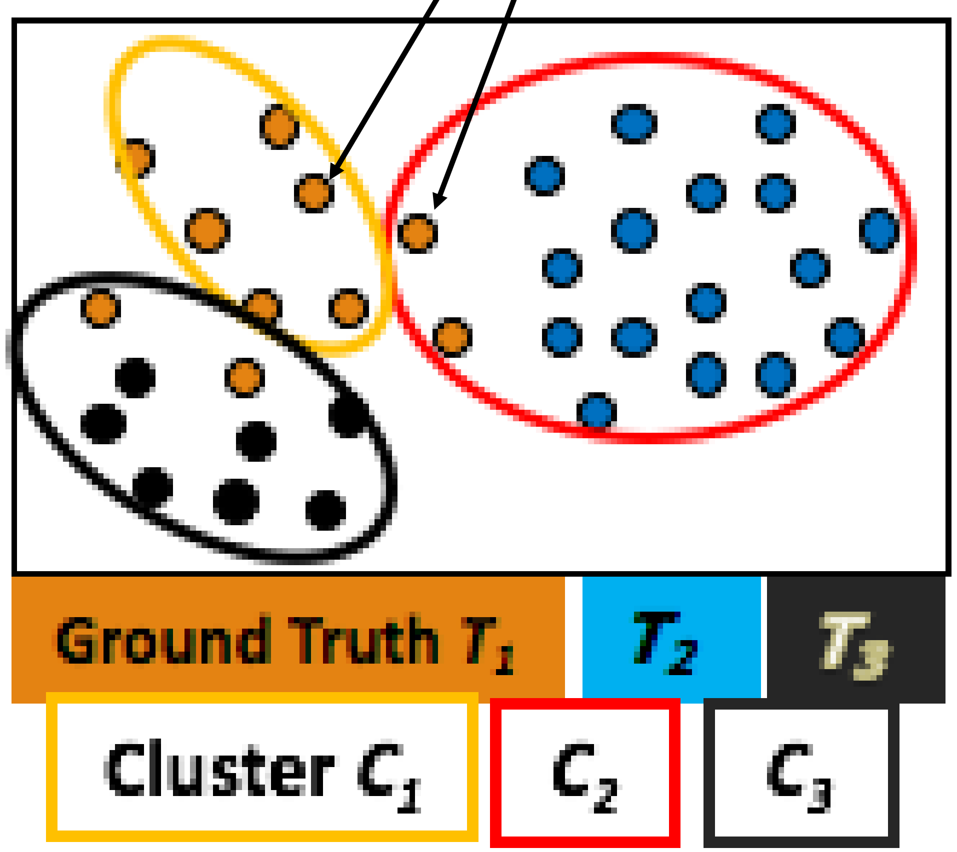
$$TP = \left|\{(\mathbf{x}_i, \mathbf{x}_j) : \; y_i = y_j \text{ and } \hat{y}_i = \hat{y}_j\}\right|$$

Same partition Same cluster



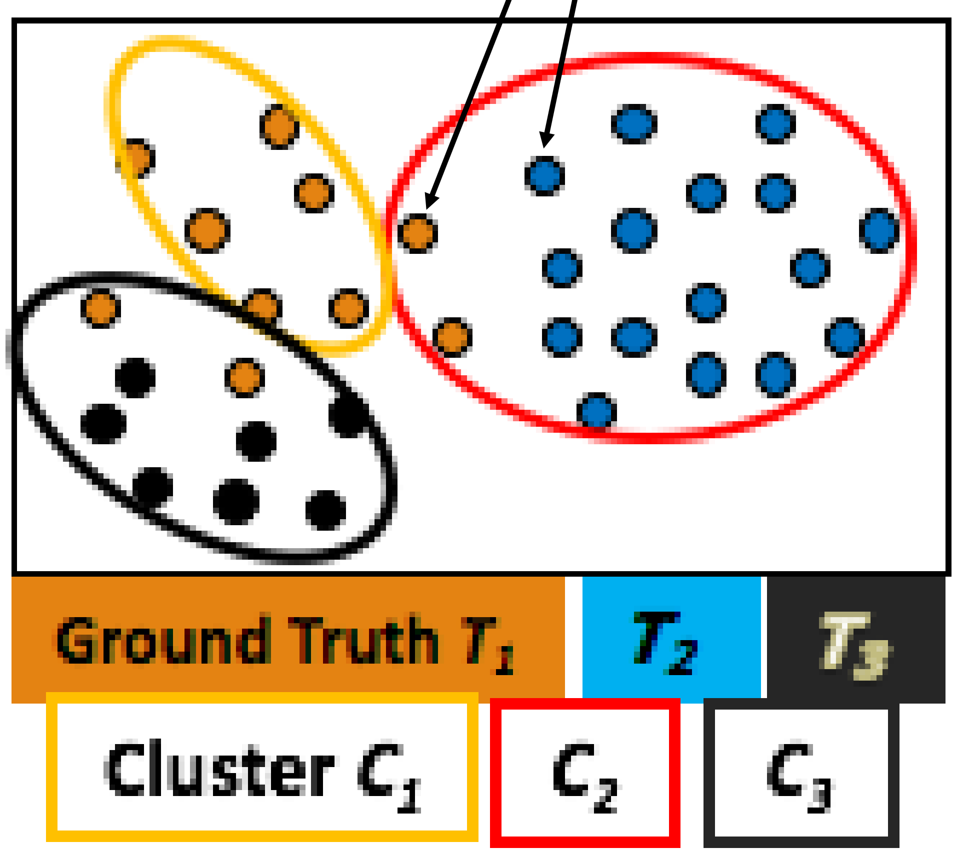
False Negatives: $\mathbf{x}_i$ and $\mathbf{x}_j$ belong to the same partition in $\mathcal{T}$, but they do not belong to the same cluster in $\mathcal{C}$. The number of all false negative pairs is given as

$$FN = \left|\{(\mathbf{x}_i, \mathbf{x}_j) : \underbrace{y_i = y_j}_{\text{Same partition}} \text{ and } \underbrace{\hat{y}_i \neq \hat{y}_j}_{\text{Different cluster}}\}\right|$$



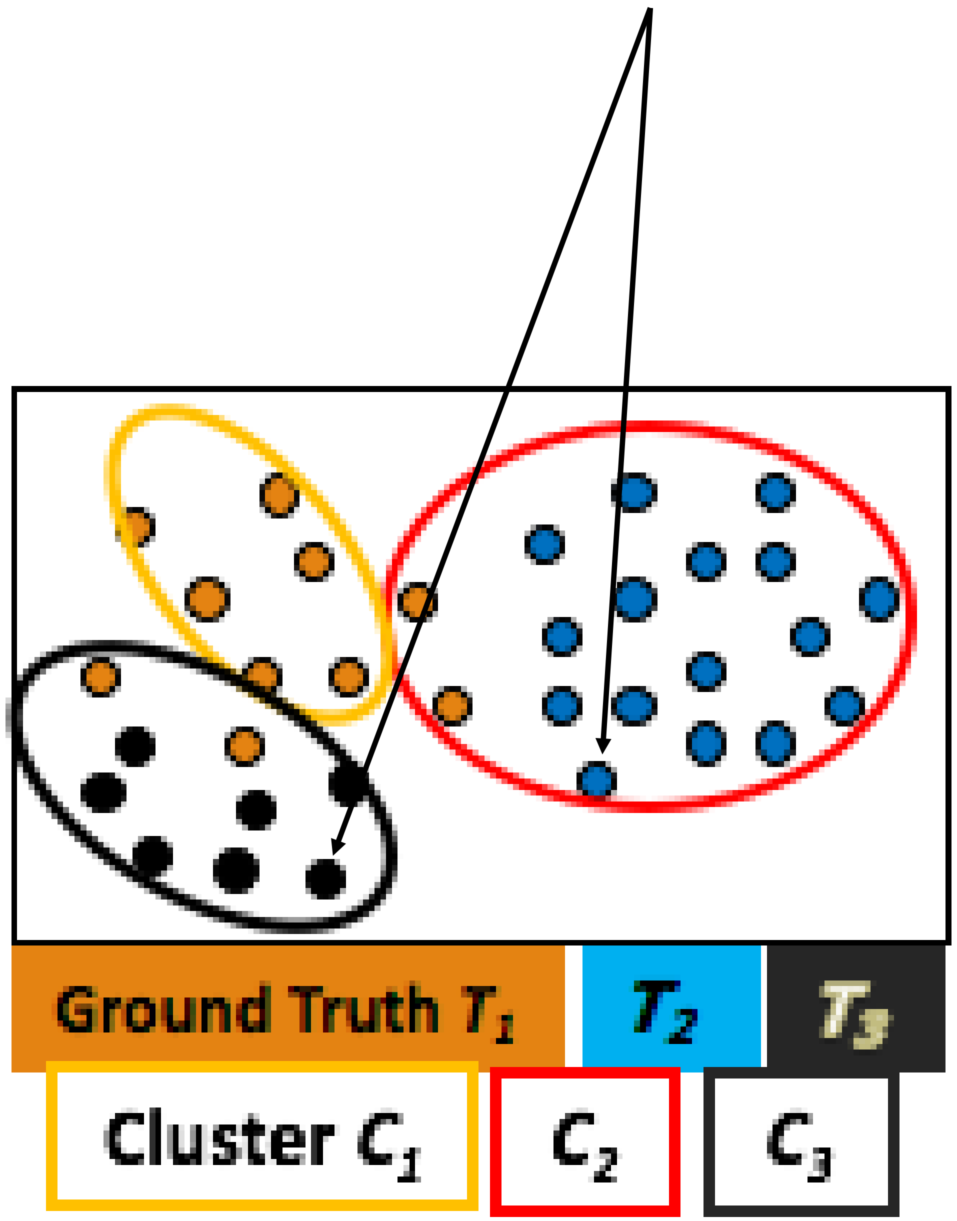
False Positives: $\mathbf{x}_i$ and $\mathbf{x}_j$ do not belong to the same partition in $\mathcal{T}$, but they do belong to the same cluster in $\mathcal{C}$. The number of false positive pairs is given as

$$FP = \left|\{(\mathbf{x}_i, \mathbf{x}_j) : \underbrace{y_i \neq y_j}_{\text{Different partition}} \text{ and } \underbrace{\hat{y}_i = \hat{y}_j}_{\text{Same cluster}}\}\right|$$



True Negatives: $\mathbf{x}_i$ and $\mathbf{x}_j$ neither belong to the same partition in $\mathcal{T}$, nor do they belong to the same cluster in $\mathcal{C}$. The number of such true negative pairs is given as

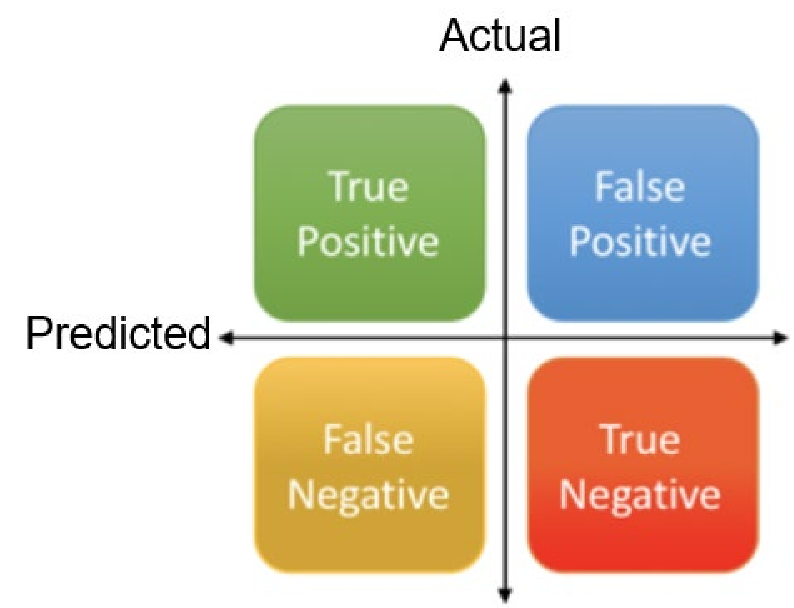
$$TN = \left|\{(\mathbf{x}_i, \mathbf{x}_j) : \underbrace{y_i \neq y_j}_{\text{Different partition}} \text{ and } \underbrace{\hat{y}_i \neq \hat{y}_j}_{\text{Different cluster}}\}\right|$$



Pairwise Measures

Because there are $N = \binom{n}{2} = \frac{n(n-1)}{2}$ pairs of points, we have the following identity:

$$N = TP + FN + FP + TN$$



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

$$\mathrm{FN} = \sum_{j=1}^{k}\binom{m_j}{2} - TP$$

$$\mathrm{FP} = \sum_{i=1}^{r}\binom{n_i}{2} - TP$$

$$\mathrm{TN} = N - (TP + FN + FP)$$

$C \backslash T$	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

$n_{12} = 20$ Points which have same Cluster one and same Partition two

Pairwise Measures

Jaccard Coefficient: measures the fraction of true positive point pairs, but after ignoring the true negative:

$$Jaccard = \frac{TP}{TP + FN + FP}$$

Perfect clustering = 1

Rand Statistic: measures the fraction of true positives and true negatives over all point pairs:

$$Rand = \frac{TP + TN}{N}$$

Perfect clustering = 1 (like accuracy)

Fowlkes-Mallows Measure: Define the overall *pairwise precision* and *pairwise recall* values for a clustering $\mathcal{C}$, as follows:

$$prec = TP/TP + FP \qquad recall = TP/TP + FN$$

The Fowlkes–Mallows (FM) measure is defined as the geometric mean of the pairwise precision and recall

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

Higher value means a better clustering

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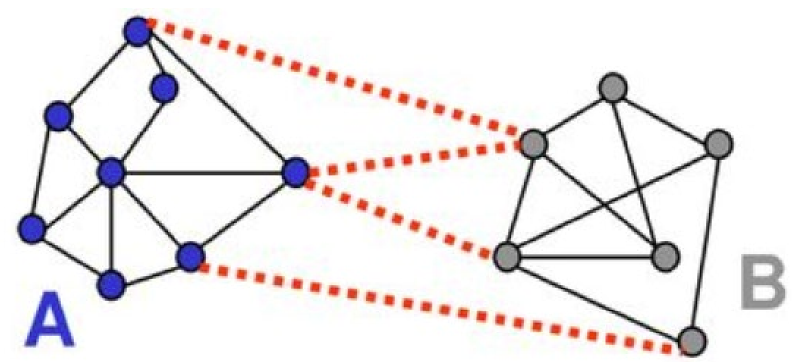
- External measures for clustering evaluation
  - Matching-based measures
  - Entropy-based measures
  - Pairwise measures
- Internal measures for clustering evaluation
  - Graph-based measures
  - Davies-Bouldin Index
  - Silhouette Coefficient

We want intra-cluster datapoints to be as close as possible to each other and inter-clusters to be as far as possible from each other

The Beta-CV Measure

- Let W be the pair-wise distance matrix for all the given points. For any two point sets S and R, we define:

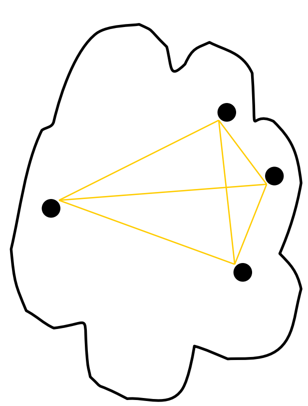


$$W(S, R) = \sum_{\mathbf{x}_i \in S} \sum_{\mathbf{x}_j \in R} w_{ij}$$

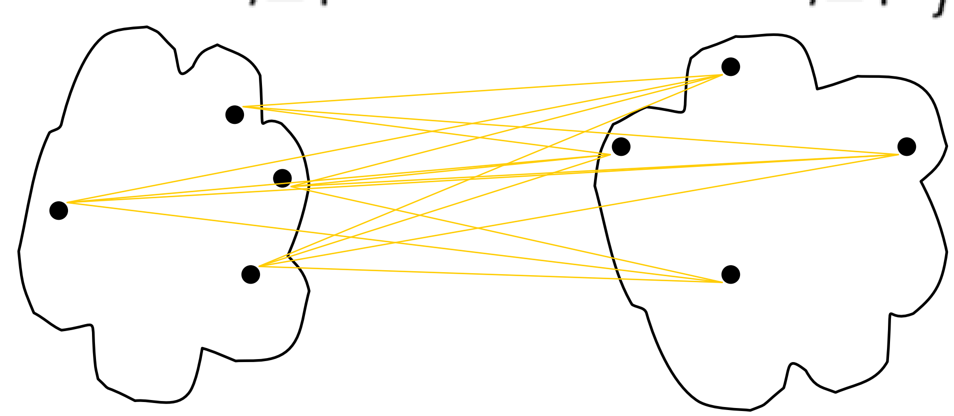
The sum of all the intracluster and intercluster weights are given as

$$W_{in} = \frac{1}{2} \sum_{i=1}^{k} W(C_i, C_i) \qquad W_{out} = \frac{1}{2} \sum_{i=1}^{k} W(C_i, \overline{C_i}) = \sum_{i=1}^{k-1} \sum_{j>i} W(C_i, C_j)$$

The distance of each point is measured two times



cohesion



separation

The Beta-CV Measure

The number of distinct intracluster and intracluster edges is given as

$$N_{in} = \sum_{i=1}^{k} \binom{n_i}{2} \qquad N_{out} = \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} n_i \cdot n_j$$

BetaCV Measure: The BetaCV measure is the ratio of the mean intracluster distance to the mean intercluster distance:

$$BetaCV = \frac{W_{in}/N_{in}}{W_{out}/N_{out}} = \frac{N_{out}}{N_{in}} \cdot \frac{W_{in}}{W_{out}} = \frac{N_{out}}{N_{in}} \frac{\sum_{i=1}^{k} W(C_i, C_i)}{\sum_{i=1}^{k} W(C_i, \overline{C_i})}$$

The smaller the BetaCV ratio, the better the clustering.

Image credit: Adriana Kovashka

Normalized Cut

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

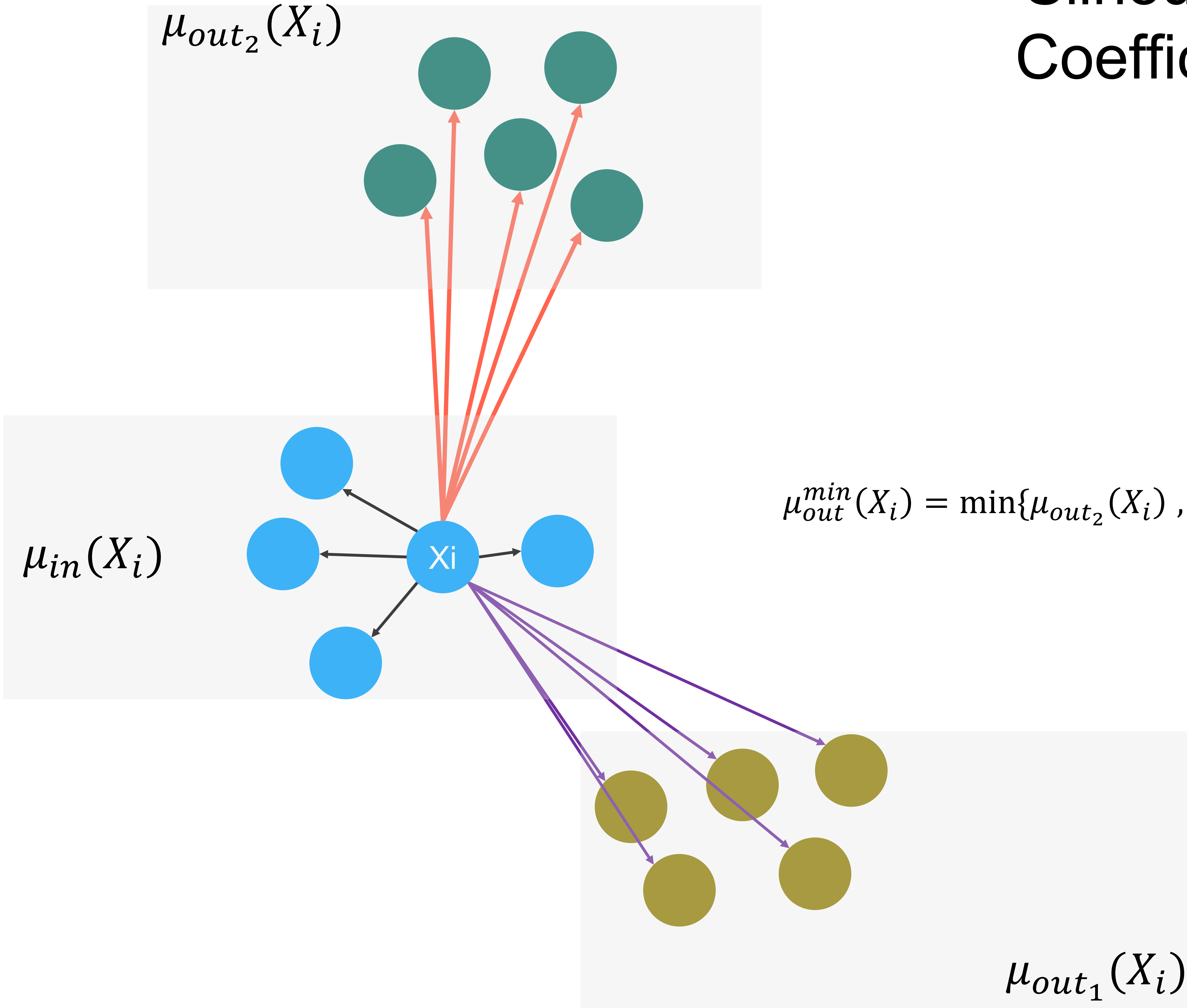
where $vol(C_i) = W(C_i, V)$ is the volume of cluster C_i

The higher normalized cut value, the better the clustering

$W(C_i, C_i)$ ↑ Intra-cluster distance

$W(C_i, \overline{C_i})$ ↑ Inter-cluster distance

Silhouette Coefficient



$$\mu_{out}^{min}(X_i) = \min\{\mu_{out_2}(X_i)\ ,\mu_{out_1}(X_i)\}$$

Silhouette Coefficient

Define the silhoutte coefficient of a point $\mathbf{x}_i$ as

$$s_i = \frac{\mu_{out}^{\min}(\mathbf{x}_i) - \mu_{in}(\mathbf{x}_i)}{\max\left\{\mu_{out}^{\min}(\mathbf{x}_i), \mu_{in}(\mathbf{x}_i)\right\}}$$

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

$$\mu_{in}(\mathbf{x}_i) = \frac{\sum_{\mathbf{x}_j \in C_{\hat{y}_i}, j \neq i} \delta(\mathbf{x}_i, \mathbf{x}_j)}{n_{\hat{y}_i} - 1}$$

and $\mu_{out}^{\min}(\mathbf{x}_i)$ is the mean of the distances from $\mathbf{x}_i$ to points in the closest cluster:

$$\mu_{out}^{\min}(\mathbf{x}_i) = \min_{j \neq \hat{y}_i} \left\{ \frac{\sum_{\mathbf{y} \in C_j} \delta(\mathbf{x}_i, \mathbf{y})}{n_j} \right\}$$

The Silhouette Coefficient for clustering C: $SC = \frac{1}{n} \sum_{i=1}^{n} s_i.$

SC close to 1 implies a good clustering (Points are close to their own clusters but far from other clusters)

The Davies-Bouldin Index

Let μ_i denote the cluster mean

$$\mu_i = \frac{1}{n_i} \sum_{\mathbf{x}_j \in C_i} \mathbf{x}_j$$

Let σ_{μ_i} denote the dispersion or spread of the points around the cluster mean

$$\sigma_{\mu_i} = \sqrt{\frac{\sum_{\mathbf{x}_j \in C_i} \delta(\mathbf{x}_j, \mu_i)^2}{n_i}} = \sqrt{var(C_i)}$$

The Davies–Bouldin measure for a pair of clusters C_i and C_j is defined as the ratio

Calculate the DB of i cluster from other clusters

$$DB_{ij} = \frac{\sigma_{\mu_i} + \sigma_{\mu_j}}{\delta(\mu_i, \mu_j)} \qquad D_i = \max_{i \neq j} DB_{ij}$$

DB_{ij} measures how compact the clusters are compared to the distance between the cluster means. The Davies–Bouldin index is then defined as

$$DB = \frac{1}{k} \sum_{i=1}^{k} D_i$$

a lower value means that the clustering is better

Summary

- External measures for clustering evaluation
  - Matching-based measures
  - Entropy-based measures
  - Pairwise measures
- Internal measures for clustering evaluation
  - Graph-based measures
  - Davies-Bouldin Index
  - Silhouette Coefficient