Lecture 23: Clustering Evaluation

April 29, 2010

Today

- Cluster Evaluation
  - Internal
    - We don't know anything about the desired labels
  - External
    - We have some information about the labels

Internal Evaluation

- Clusters have been identified.
- How successful a partitioning of the data set was constructed through clustering?

- Internal measures have the quality that they can be directly optimized.

Intercluster variability

- How far is a point from its cluster centroid

$$J(x|\theta) = \frac{1}{N}\sum_i ||x_i - c_i||^2$$

- Intuition: every point assigned to a cluster should be closer to the center of that cluster than any other cluster
- K-means optimizes this measure.

Model Likelihood

$$p(x|\theta)$$

- Intuition: the model that fits the data best represents the best clustering
- Requires a probabilistic model.
- Can be included in AIC and BIC measures to limit the number of parameters.
- GMM style: $p(x|\theta) = \sum_k \pi_k p(x|\mu_k, \Sigma_k)$

Point similarity vs. Cluster similarity

$$\frac{1}{2}\sum_{ij} sim(x_i, x_j)(c_i - c_j)^2$$

- Intuition: two points that are similar should be in the same cluster
- Spectral Clustering optimizes this function.

Internal Cluster Measures

- Which cluster measure is best?
  - Centroid distance
  - Model likelihood
  - Point distance
- It depends on the data and the task.

External Cluster Evaluation

- If you have a little bit of labeled data, unsupervised (clustering) techniques can be evaluated using this knowledge.

- Assume for a subset of the data points, you have class labels.
- How can we evaluate the success of the clustering?

External Cluster Evaluation

- Can't we use Accuracy?
  - or "Why is this hard?"
- The number of clusters may not equal the number of classes.
- It may be difficult to assign a class to a cluster.

Some principles.

- Homogeneity
  - Each cluster should include members of as few classes as possible
- Completeness
  - Each class should be represented in as few clusters as possible.

Some approaches

- Purity

$$Purity = \sum_{r=1}^{k} \frac{1}{n} \max_{i}(n_r^i)$$

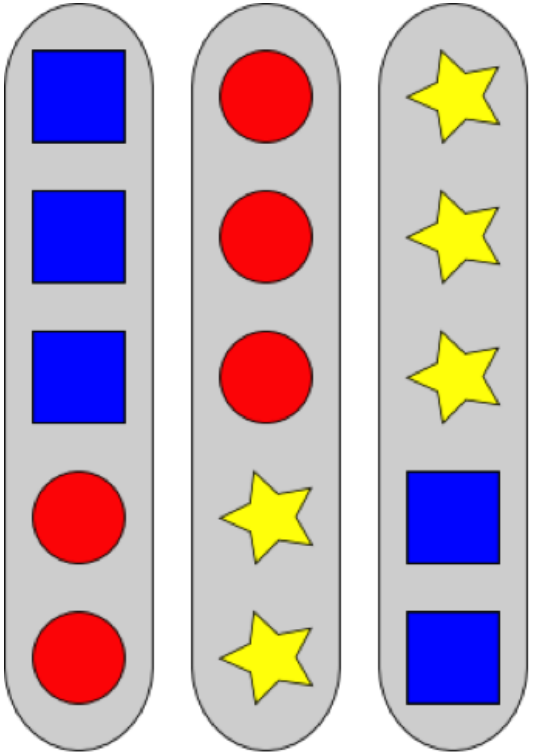
points of class *i* in cluster *r*

- F-measure
  - Cluster definitions of Precision and Recall
  - Combined using harmonic mean as in traditional f-measure

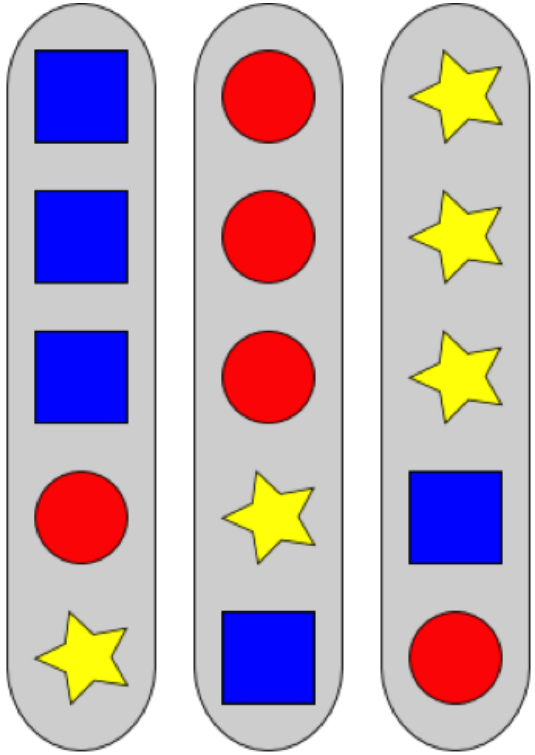
$$R(c_i, k_j) = \frac{n_{ij}}{|c_i|}$$

$$P(c_i, k_j) = \frac{n_{ij}}{|k_j|}$$

The problem of matching

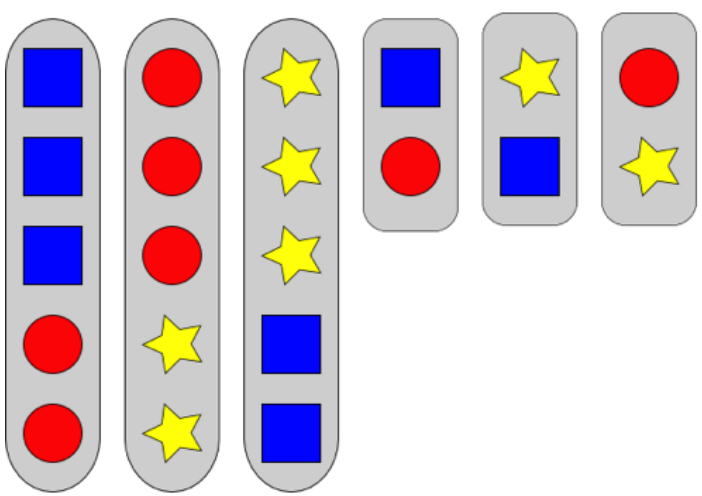


F-measure: 0.6

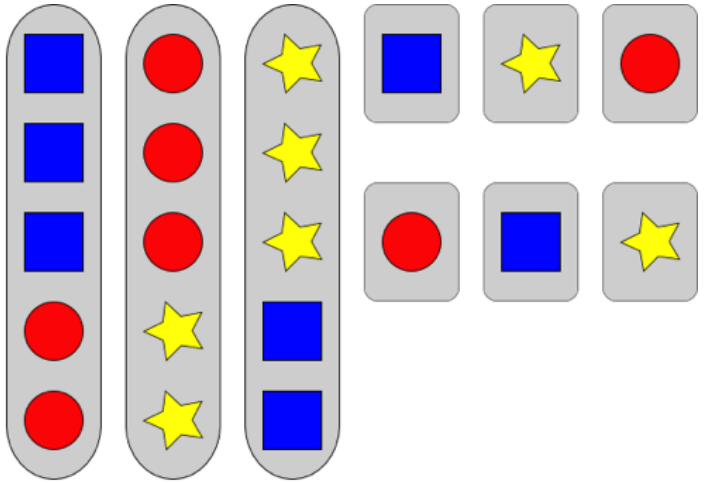


F-measure: 0.6

The problem of matching



F-measure: 0.5



F-measure: 0.5

V-Measure

- Conditional Entropy based measure to explicitly calculate homogeneity and completeness.

$$V_\beta = \frac{(1+\beta) * h * c}{(\beta * h) + c}$$

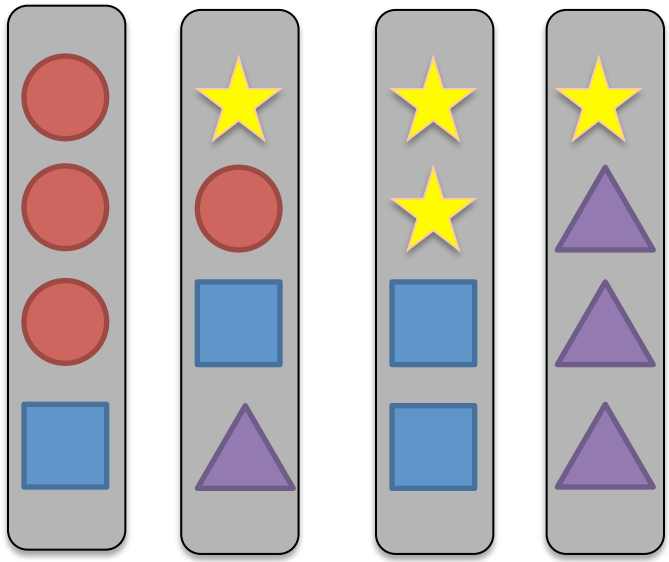
$$h = \begin{cases} 1 & \text{if } H(C,K) = 0 \\ 1 - \frac{H(C|K)}{H(C)} & \text{else} \end{cases}$$

$$c = \begin{cases} 1 & \text{if } H(K,C) = 0 \\ 1 - \frac{H(K|C)}{H(K)} & \text{else} \end{cases}$$

Contingency Matrix

- Want to know how much the introduction of clusters is improving the information about the class distribution.

3	1			4
	1	2	1	4
1	1	2		4
	1		3	4
4	4	4	4	



Entropy

- Entropy calculates the amount of “information” in a distribution.
- Wide distributions have a lot of information
- Narrow distributions have very little
- Based on Shannon’s limit of the number of bits required to transmit a distribution
- Calculation of entropy:

$$H(x) = -\sum_i p(x_i) \log_2 p(x_i)$$

Example Calculation of Entropy

$$x = \begin{bmatrix} \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{bmatrix}$$

$$H(x) = -\frac{1}{4}\log\frac{1}{4} - \frac{1}{4}\log\frac{1}{4} - \frac{1}{4}\log\frac{1}{4} - \frac{1}{4}\log\frac{1}{4}$$

$$\begin{aligned} H(x) &= -\frac{1}{4}(-2) - \frac{1}{4}(-2) - \frac{1}{4}(-2) - \frac{1}{4}(-2) \\ &= 2 \end{aligned}$$

Example Calculation of Entropy

$$x = \begin{bmatrix} \frac{4}{10} & \frac{4}{10} & \frac{1}{10} & \frac{1}{10} \end{bmatrix}$$

$$\begin{aligned} H(x) &= -\frac{4}{10}\log\frac{4}{10} - \frac{4}{10}\log\frac{4}{10} - \frac{1}{10}\log\frac{1}{10} - \frac{1}{10}\log\frac{1}{10} \\ &= -\frac{4}{10}(-1.32) - \frac{4}{10}(-1.32) - \frac{1}{10}(-3.32) - \frac{1}{10}(-3.32) \\ &= 1.72 \end{aligned}$$

Pair Based Measures

- Statistics over every pair of items.
  - SS – same cluster, same class
  - SD – same cluster, different class
  - DS – different cluster, same class
  - DD – different cluster different class
- These can be arranged in a contingency matrix similar to when accuracy is constructed.

Pair Based Measures

- Rand:

$$Rand = \frac{SS + DD}{SS + SD + DS + DD}$$

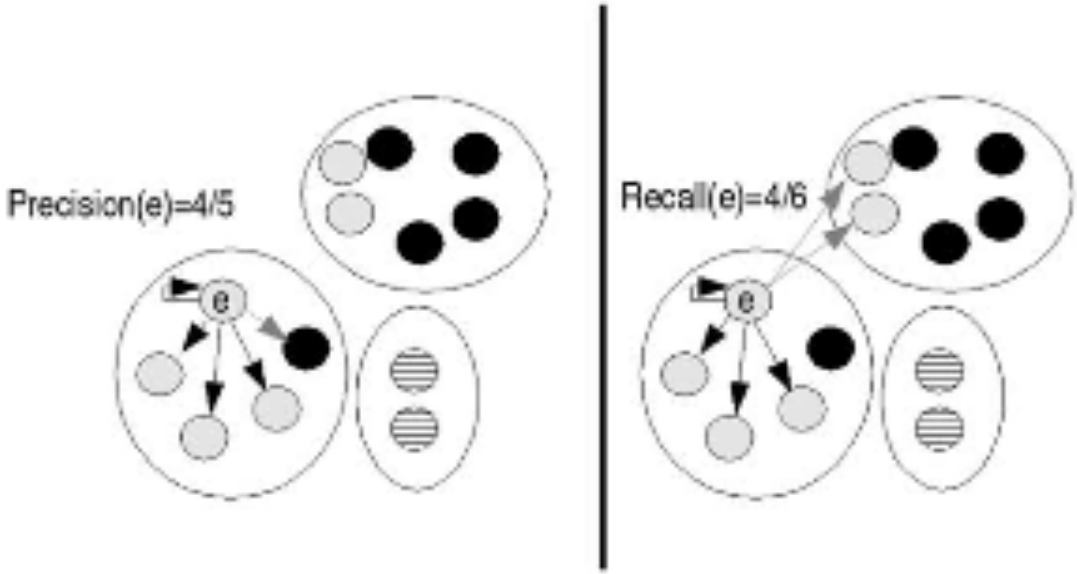
- Jaccard

$$Jaccard = \frac{SS}{SS + SD + DS}$$

- Folkes-Mallow

$$FM = \sqrt{\frac{SS}{SS + SD} \cdot \frac{SS}{SS + DS}}$$

B-cubed



$$Precision = \frac{\sum_i Precision(e)}{n} \qquad Recall = \frac{\sum_i Recall(e)}{n}$$

- Similar to pair based counting systems, B-cubed calculates an element by element precision and recall.

External Evaluation Measures

- There are many choices.

- Some should almost certainly never be used
  - Purity
  - F-measure
- Others can be used based on task or other preferences
  - V-Measure
  - VI
  - B-Cubed

Next Time

- Project Presentations
  - The schedule has 15 minutes per presentation.
  - This includes transition to the next speaker, and questions.
  - Prepare for 10 minutes.
- Course Evaluations

Thank you