Unsupervised Learning: Model Selection and Evaluation

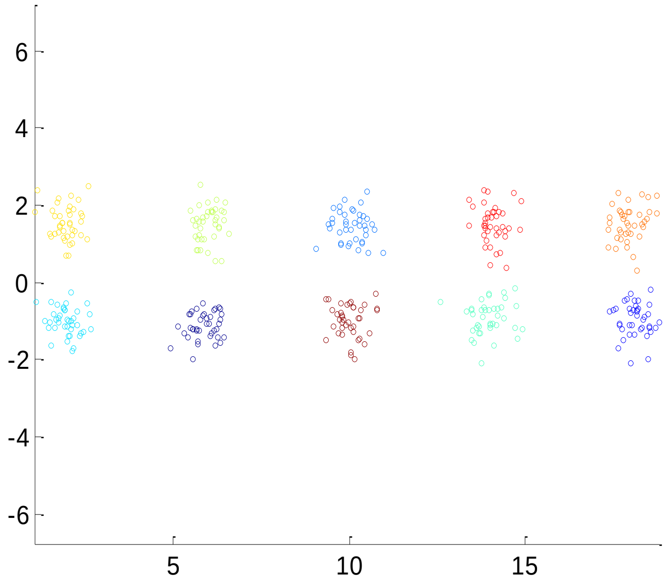
CS-534

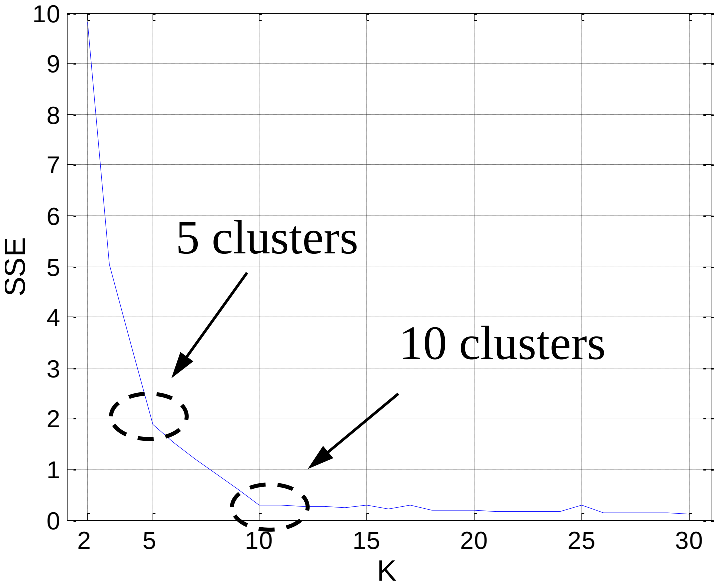
Selecting k: A Model Selection Problem

- Each choice of k corresponds to a different statistical model for the data
- Model selection searches for a model (a choice of k) that gives us the best fit of the training data
  - Penalty method
  - Cross-validation method
  - Model selection methods can also be used to make other model decisions such as choosing among different ways of constraining Σ

Selecting k: heuristic approaches

- For kmeans, plot the sum of squared error for different k values
  - SSE will monotonically decrease as we increase k
  - Knee points on the curve suggest possible candidates for k





Penalty Method: Bayesian Information Criterion

- Based on Bayesian Model Selection
  - Determine the range of k values to consider $1 \leq k \leq K_{max}$
  - Apply EM to learn a maximum likelihood fitting of the Gaussian mixture model for each possible value of *k*
  - Choose *k* that maximizes BIC

# of data points

$$\underbrace{2l_{\mathcal{M}}(x,\hat{\theta})}_{\text{Loglikelihood of the resulting Gaussian Mixture Model}} - m_{\mathcal{M}} \log(n) \equiv \text{BIC}$$

Loglikelihood of the resulting Gaussian Mixture Model

# of parameters to be estimated in *M*

  - Given two estimated models, the model with higher BIC is preferred
  - Larger k increases the likelihood, but will also cause the second term to increase
  - Often observed to be biased toward less complex model
  - Similar method: $\text{AIC} = 2l_m - 2m_M$, which penalize complex model less severely

Cross-validation Likelihood
(Smyth 1998)

- The likelihood of the training data will always increase as we increase k
  - more clusters, more flexibility leads to better fitting of the data
- Use cross-validation
  - For each fold, learn the GMM model using the training data
  - Compute the log-likelihood of the learned model on the remaining fold as test data

How to Evaluate Clustering?

- By user interpretation
  - does a document cluster seem to correspond to a specific topic?
- Internal criterion – a good clustering will produce high quality clusters:
  - high intra-cluster similarity
  - low inter-cluster similarity

  - The measured quality of a clustering depends on both the object representation and the similarity measure used

External indexes

If true class labels (*ground truth*) are known, the validity of a clustering can be verified by comparing the class labels and clustering labels.

$$
\begin{array}{|c|c}
\hline N & \cdot \\
\hline \cdot & n_{\cdot\cdot}
\end{array}
=
\begin{array}{|cccc|c}
\hline
n_{11} & n_{12} & \cdots & n_{1l} & n_{1\cdot} \\
n_{21} & n_{22} & \cdots & n_{2l} & n_{2\cdot} \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
n_{k1} & n_{k2} & \cdots & n_{kl} & n_{k\cdot} \\
\hline
n_{\cdot 1} & n_{\cdot 2} & \cdots & n_{\cdot l} & n_{\cdot\cdot}
\end{array}
$$

n_{ij} = number of objects in class *i* and cluster *j*

Rand Index and Normalized Rand Index

- Given partition (*P*) and ground truth (*G*), measure the number of vector pairs that are:

  a: in the same class <u>both</u> in *P* and *G*.
  b: in the same class in *P*, but different classes in *G*.
  c: in different classes in *P*, but in the same class in *G*.
  d: in different classes <u>both</u> in *P* and *G*.

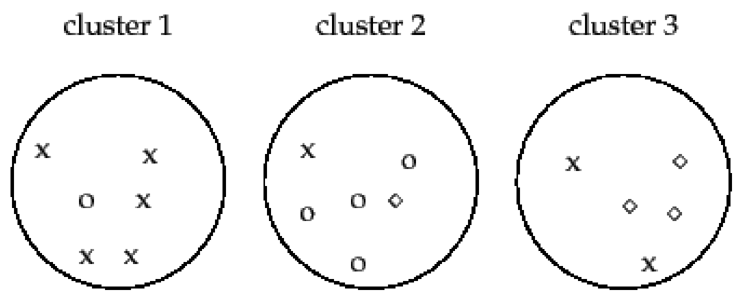
$$R = \frac{a+d}{a+b+c+d}$$

- Adjusted rand index: corrected-for-chance version of rand index
  - Compare to the expectation of the index assuming a random partition of the same cluster sizes

$$ARI = \frac{Index - ExpectedR}{MaxIndex - ExpectedR} = \frac{\sum_{i,j}\binom{n_{ij}}{2} - \left[\sum_i \binom{n_{i.}}{2} \sum_j \binom{n_{.j}}{2}\right] / \binom{n}{2}}{\frac{1}{2}\left[\sum_i \binom{n_{i.}}{2} + \sum_j \binom{n_{.j}}{2}\right] - \left[\sum_i \binom{n_{i.}}{2} \sum_j \binom{n_{.j}}{2}\right] / \binom{n}{2}}$$

Purity and Normalized Mutual Information

- Purity



► **Figure 16.1** Purity as an external evaluation criterion for cluster quality. Majority class and number of members of the majority class for the three clusters are: x, 5 (cluster 1); o, 4 (cluster 2); and ⋄, 3 (cluster 3). Purity is $(1/17) \times (5 + 4 + 3) \approx 0.71$.

- Normalized Mutual Information

Mutual info:

cla1	cla2	cla3
50	50	50

Cluster 1		
40	8	10

Cluster 2		
6	30	15

Cluster 3		
4	12	25

$$I(Class, Clust) = H(Class) - H(Class|Clust)$$

$$NMI = \frac{2I(Class, Clust)}{H(Clust) + H(Class)}$$