Identify Leaf clusters

Addison James, Bin Zhuo, Feifei Lei, Nandhita Narendra Babu

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Contents

Overview

- To identify the leaf clusters from leaf data set
- Leaf dataset
    - Collection of shape and texture features extracted from digital images of leaf specimens
    - A total of 40 different plant species
    - Only 30 of those were present in the data provided
    - 340 observations

Methods

"All methods are concerned with using the inherent structures in the data to best organize the data into groups of maximum commonality"
- Jasonb in "A Tour of Machine Learning Algorithms"

- **K-means Clustering**
  To make 30 clusters to see how well this approach recovers the real data
- **Model-based clustering**
  To group the leaves at higher level

K-Means Clustering

Method Description

- Definition $\rightarrow$ Assigning n observations into k clusters
- Requires to specify the number of clusters k to extract
- Similarity criterion $\rightarrow$ proximity to the mean of each cluster
- Assignment method $\rightarrow$ minimize euclidean distance from the data to the means of the clusters

Algorithm Description

1. Set Initial Cluster Means
2. Assign each datum to the cluster with the nearest mean
3. Calculate the new mean of each cluster
4. Repeat steps 2-3 until convergence

Procedure

- function *kmeans* : To cluster leaves into species
- $k = 30$ clusters $\rightarrow$ cluster all the observations into 30 separate species based on the 14 covariates available
- Covariates : eccentricity, aspect ratio, elongation, solidity, stochastic convexity, isoperimetric factor, maximal indentation depth, lobedness, average intensity, average contrast, smoothness, third moment, uniformity, and entropy

K-means Clustering result

Two possible solutions

- First solution
  - examine each cluster and assigns a species number to each cluster based on the most frequent species in the cluster
  - can fail to create a one-to-one relationship between the species and cluster $\rightarrow$ there may be a tie or two different clusters may be assigned to the same species
- Second solution
  - examine each species and assign the species to the clusters, but reversing the role of clusters and species

K-means Clustering result

- Result from First Method
  - 138 of the 340 observations (41%) ended up in the correct cluster
  - successfully assigned 19 of the 30 clusters (63%) to a species
- Result from Second Method
  - less optimistic evaluation
  - 126 observations were correctly clustered (37%)
  - 17 of the 30 species were assigned a cluster (57%)
  - poor job of grouping leaves of the same species based on the known covariates

Model-based Clustering

Method description

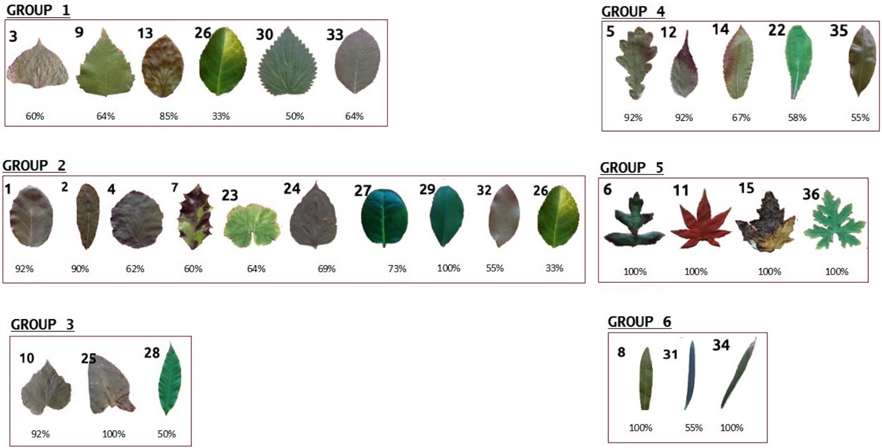
- Basic idea: Clustering as probability estimation
- One model for each cluster
- Generative model:
    - Probability of selecting a cluster
    - Probability of generating an object in cluster
- Use EM algorithm

Procedure

- Covariance parameterization and number of clusters are selected via BIC
- Clustering using normal mixture modeling via EM algorithm
- *Mclust* function
  - Selects the optimal model according to BIC for EM initialized by Guassian Mixture Models
  - Chooses the model and number of clusters with the largest BIC

Model-based clustering results

Optimal cluster number $\rightarrow$ 6



Assumptions/Limitations and Scalability

Assumption/Limitations

- Assumptions
  - Normality
- Limitations
  - K-means Clustering
    - comparable size of clusters
  - Model-based clustering
    - provides only 10 of the 14 possible variance-covariance structures
    - Cannot handle 'NA' problem

Scalability

- k-Means is faster than hierarchical clustering
- function *mclust* is able to cope with large datasets
- Mclust can use sampled data in the hierarchical phase before applying EM to extend the method to larger datasets

Questions ?

EM Algorithm Description

EM Algorithm

- **Initialization**: Choose means at random
- **E step**:
    - For all points and means, compute P(point|mean)
    - P(mean|point) = P(mean) P(point|mean) / P(point)
- **M step**:
    - Each mean = Weighted avg. of points
    - Weight = Prob(mean|point)
- Repeat until convergence
- Guaranteed to converge to local optimum