Choosing the Number of Clusters in Monothetic Clustering

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Clustering

- Clustering algorithms attempt to group subjects so that the dissimilarity within clusters is smallest while the between cluster dissimilarities are largest.
  - Q = number of response variables, n = sample size, y_{iq} is the i^{th} observation on variable q.
  - n objects in Ω, with partition $P_J = C_1, \ldots, C_J$ the J-cluster partition of Ω.
- The choice of J impacts the group memberships and thus the interpretation of the results.
  - J too small puts "unlike" subjects together.
  - J too large splits observations that should be together.
- Ruspini (1970) used a data set with 70 observations on two variables to demonstrate clustering techniques.

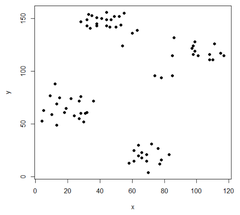


Figure: Ruspini data set

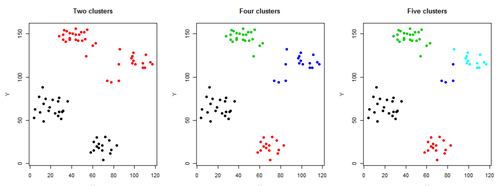


Figure: Different possible cluster solutions for Ruspini's data.

Research Question

How many clusters should observations be classified into when using monothetic clustering?

- Goal: Objective numerical measures for selecting the "correct" number of clusters.

Monothetic Cluster Analysis (Chavent, 1998)

- Hierarchical, recursive partitioning of multivariate responses based on binary decision rules built from individual response variables.
- Inspired by Regression Trees (see Hastie et al., 2009).
  - Search for splits from each response variable that provide the best split of the multivariate responses (measured with global criterion called inertia).
  - Recursively apply to each sub-partition, recording splitting rules that define clusters.
  - Generates a set of binary rules for cluster membership ("monothetic").
- Defining within cluster inertia: total variability around the cluster mean.
  - If Euclidean distance is being used, inertia for cluster j,

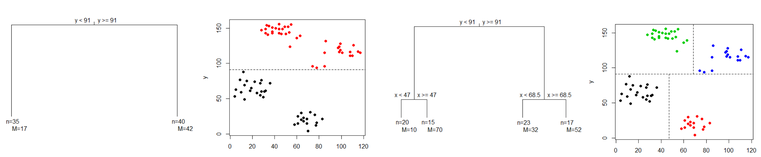
$$I(C_j) = \sum_{i \in \text{Cluster}_j} \sum_{q=1}^{Q} (y_{iq} - \overline{y}_{\cdot q})^2.$$

  - Choose the bipartition for cluster C to maximize the difference in inertia,

$$I(C) - I(C_1) - I(C_2).$$

  - Recursively apply to each sub-partition.
  - Equivalence of distances for all observations within cluster and within group variation (p. 388, James et al., 2013) is exploited to use inertia with any dissimilarity matrix.
- An R package `MonoClust` is under development - go to `http://tinyurl.com/MonoClust`.

Monothetic Cluster Analysis of Ruspini Data



(a) One split, two clusters (b) Three splits, four clusters

Figure: Binary partitioning tree with maps of optimal splits.

- For four clusters:
  - Cluster 1: y below 91 and x below 47 and Cluster 2: y below 91 and x above 47
  - Cluster 3: y over 91 and x below 68.5 and Cluster 4: y over 91 and x over 68.5

Some Popular Metrics for Choosing Number of Clusters

1. Average silhouette width (AW) (Rousseeuw, 1987)
   - The silhouette width is a measure of how "comfortable" an observation is in the cluster it resides in.
     - Between 0 and 1 if "happiest" in existing cluster.
     - 0 if ambivalent about cluster membership vs. next closest cluster.
     - Between -1 and 0 if observation "wants to leave" current cluster.
   - The average silhouette width is mean of all n silhouette widths.
   - Select cluster solution size J that has maximum average silhouette width.
   - It is not defined for $J = 1$ so cannot select a single cluster solution.
2. Calinski and Harabasz (CH)'s pseudo-F (Calinski and Harabasz, 1974)
   - Choose J to maximize variation between clusters relative to variation within clusters.
   - Use pseudo-F= $\frac{B(J)/(J-1)}{W(J)/(n-J)}$ with $B(J)$ the between cluster sums of squares (possibly from dissimilarities) and $W(J)$ the within cluster sums of squares.
   - It is not defined for $J = 1$ so cannot select a single cluster solution.
3. Many others exist: See Milligan and Cooper (1985) and `NbClust` (Charrad et al., 2014) in R.

Proposed Methods for Choosing Number of Clusters

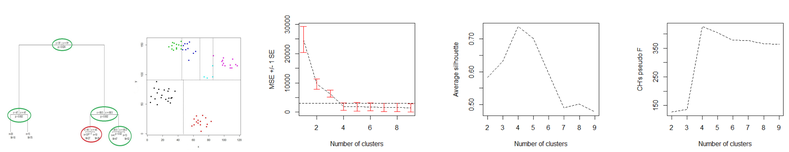
1. M-fold Cross-Validation
   - Based on ideas for pruning regression trees (Breiman et al., 1984).
   - Randomly divide data set into M equal-sized subsets, withhold a subset, and use the rest for training the method.
   - Compute a measure of prediction error for the m^{th} set of withheld observations, such as $MSE_m = \frac{1}{n_m} \sum_{q=1}^{Q} \sum_{i \in m} (y_{iq} - \hat{y}_{iq})^2$ where $\hat{y}_{iq}$ are the predicted responses.
   - Cross-validation based estimate of the error for the J cluster solution is

$$CV_J = \frac{1}{M} \sum_{m=1}^{M} MSE_m.$$

   - CV-based selection rules:
     1. Choose J that provides the smallest CV_J (`minimum CV rule`).
     2. Choose solution that provides simplest solution within 1 standard error of the minimum (`1 SE rule`) where $SE = \sqrt{\frac{1}{M-1} \sum_{i=1}^{M} (MSE_i - \overline{MSE})^2}$.
   - Monothetic clustering is one of the few clustering algorithms that provides a clear prediction rule – use the binary rules to assign a new observation to a cluster.
     - Then use cluster means to generate predicted response $\hat{y}_{iq}$.
     - Implemented as `predict` for MonoClust class (`predict.MonoClust`).
   - Open question: How does the maximum size of the tree explored impact 1SE rule results?
2. Hypothesis tests at each bipartition in the monothetic cluster solution
   - Based on ideas from conditional inference trees (R package `party`, Hothorn et al., 2006).
     - Grow tree until a split has a p-value over pre-determined threshold (say α of 0.01 or 0.05), adjusting p-values based on depth in tree.
   - Test assesses H_0: *no difference in two groups at node* using permutations of observations and pseudo-F test statistic (as defined in perMANOVA in Anderson, 2001).
     - Available in `adonis` in `vegan` package (Oksanen et. al., 2015).
   - P-values are Bonferroni adjusted for number of tests required to get to level of tree,

$$\text{P-value}_{adj} = \text{depth} \times \frac{\text{No. of } (F_{perm} \geq F_{observed})}{\text{No. of perm}}.$$

   - Problem with applying regular tests to monothetic clustering:
     - Selected split is always the most extreme result possible on variable that defined the bipartition.
     - Potential solution: Only use variation from the Q-1 variables not used to define two groups in test statistic.
       - Differences will be detected if the binary split is useful on other variables.
       - Can not be applied to clustering when Q=1.
   - Implemented as `perm.test` which adds p-value information to the tree-display with `auto.pick` argument to automatically prune the tree based on a selected threshold.



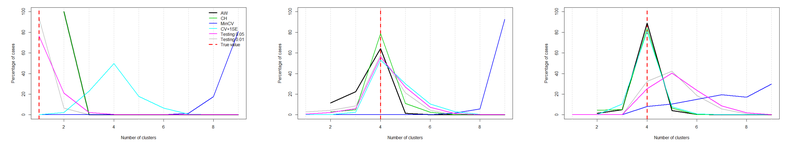
(a) Hypothesis testing: selects 5 clusters (b) 10-fold CV: selects max (minCV), 4 (1SE) (c) Ave silhouette: selects 4 clusters (d) CH's pseudo-F: selects 4 clusters

Figure: Criteria results for monothetic cluster analysis of Ruspini's data.

Simulation Study: Three scenarios considered, L^2 distances

1. *Null model with 10 dimensions:* J=1, Q=10, $y_{iq} \sim U(-1, 1)$
2. *Four clusters in 3 dimensions:* $J = 4$, Q=3, $\mu_j \sim N(0, 5\text{I}_3)$ and $\mathbf{y}_i \sim N(\mu_j, \text{I}_3)$.
   - Cluster sizes are randomly chosen from either 25 or 50 observations.
   - Only samples where distance between two closest observations in clusters is at least 2 units are analyzed.
3. *Four clusters in 10 dimensions:* $J = 4$, Q=10, $\mu_j \sim N(0, 1.9\text{I}_{10})$ and $\mathbf{y}_i \sim N(\mu_j, \text{I}_{10})$
   - Cluster sizes randomly chosen from 25 or 50 observations and distance between clusters ≥ 2 units.

Simulation Study: Results of 500 simulations



(a) Scenario 1 (b) Scenario 2 (c) Scenario 3

Figure: Simulation results

- Only hypothesis testing method works well when $J = 1$.
  - It is quite successful when $\alpha = 0.01$ at correctly preventing a search past the root node.
  - With $\alpha = 0.01$, the $J = 1$ solution is rejected 6% of the time – type I error rates inflated because assessing splits that are optimal globally from given choices.
    - Rejection rates were much higher with moderate Q when all variables were included in test statistic.
- Hypothesis testing using the more conservative α value provided more correct results but hypothesis testing struggled with larger Q.
- The minimum CV value is often the largest number of clusters considered – suggests criterion does not provide much penalty for over-fitting.
- 1SE rule with CV is much better than minimum CV and close to other methods in performance except in *Scenario 1*.
  - Some mistakes in *Scenarios 2* and *3* might be due to var(CV) in different random partitions.

Conclusions

- Some methods, such as CH and AW, cannot select one cluster so can't help researcher decide between one versus more than one cluster.
  - Clustering algorithms always generate groups – and these methods can't assess whether any should be found.
- Both CV and p-value based methods are attractive as they provide direct information about utility of single cluster versus other sizes.
  - Hypothesis testing can work but seems to suffer as the dimension of the data set grows.
  - CV results vary in repeated application with same data; variability may be impacting selection performance.
- The speed of `MonoClust` depends largely on the number of dimensions.
- CV is slowest of methods considered because of M re-fittings of monothetic cluster solution.
- Permutation testing is fast due to `adonis` function and only single monothetic cluster solution required.
- Recommendations for finding number of clusters in monothetic clustering:
  - Use permutation test to assess evidence for more than one cluster using modified test statistic and small α.
  - If initial p-value is small, use pseudo-F maximization (CH) to find correct size of cluster solution.
  - Use predict function to classify and generate predictions for new observations.
  - If using CV-based methods, use 1SE rule and consider multiple runs of CV splitting process to identify the most commonly selected optimal cluster size.

Future Work

- Finalize the R package and assess criteria in more situations with changing variability.
- Include GAP (Tibshirani et al., 2001) and other criteria in comparisons - some may work better for monothetic clustering than others and provide $J = 1$ selection possibility.
- Permutation tests could be used in other hierarchical clustering techniques, assessing evidence of need for divisions from top of tree down.
  - See `pvclust` (Suzuki et al., 2006) for bootstrap-based p-value approach with regular hierarchical clustering.

Acknowledgments

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References, copy of poster, and MonoClust code available in github repository: `http://tinyurl.com/MonoClust`.