Interactive Clustering
Overview and Tools

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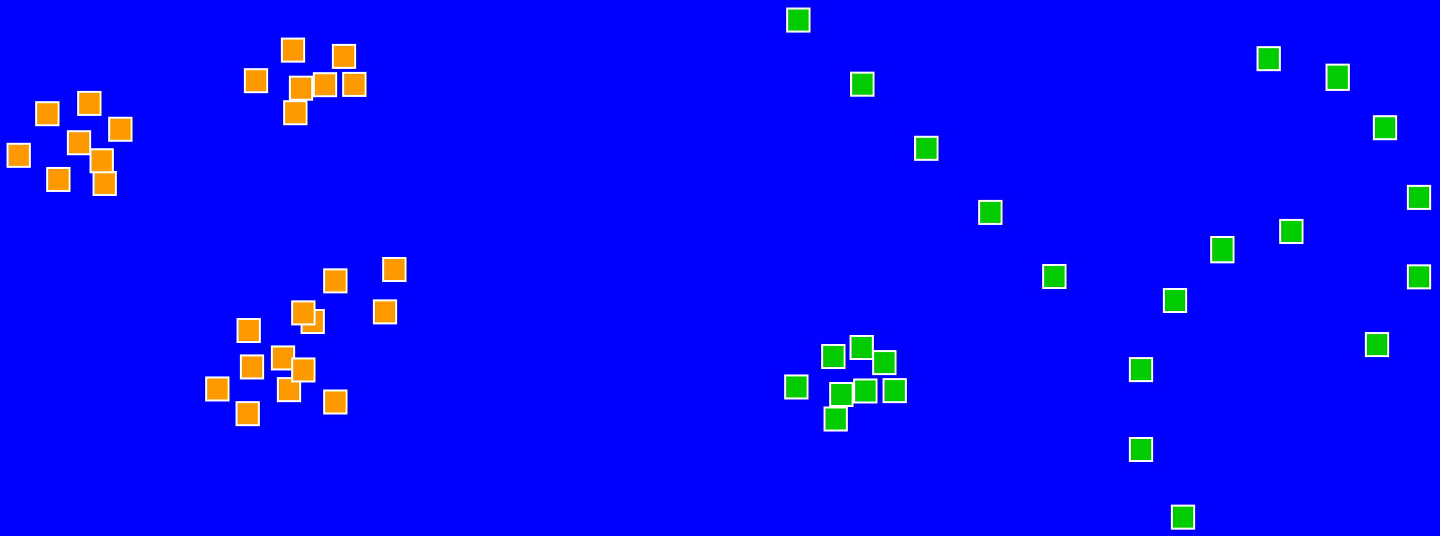
Overview

1. Finding groups in data
2. Interactive data analysis
3. Enlarging the problem
4. Putting it together
5. Software modelling (illustration)
6. Summary

1.Finding groups in data

- Objects to be grouped together
  - locations
  - pairwise (dis)similarities
- Applications:
  - Web documents as objects to be grouped
  - Building groups to use later as classification
  - Building groups to serve as templates
  - Building groups to understand/model



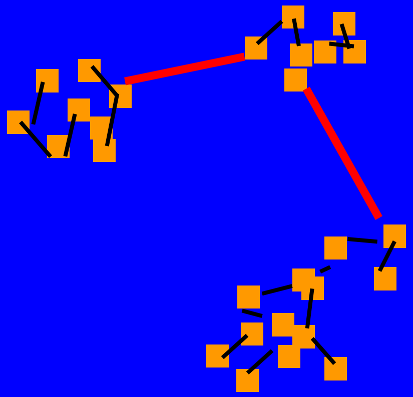
Group definition (like with like)

- homogeneous vs heterogeneous
- part of pattern

group definition is a problem

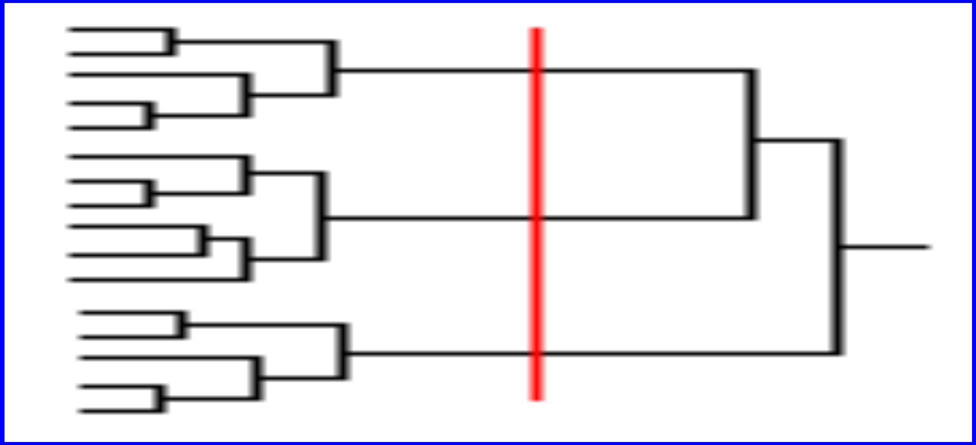
Clustering approaches

- Agglomerative (near points/clusters are joined)
  - Single linkage
  - Complete linkage
  - Average linkage



- Recursive splitting
  - e.g. minimal spanning tree

Cluster hierarchies

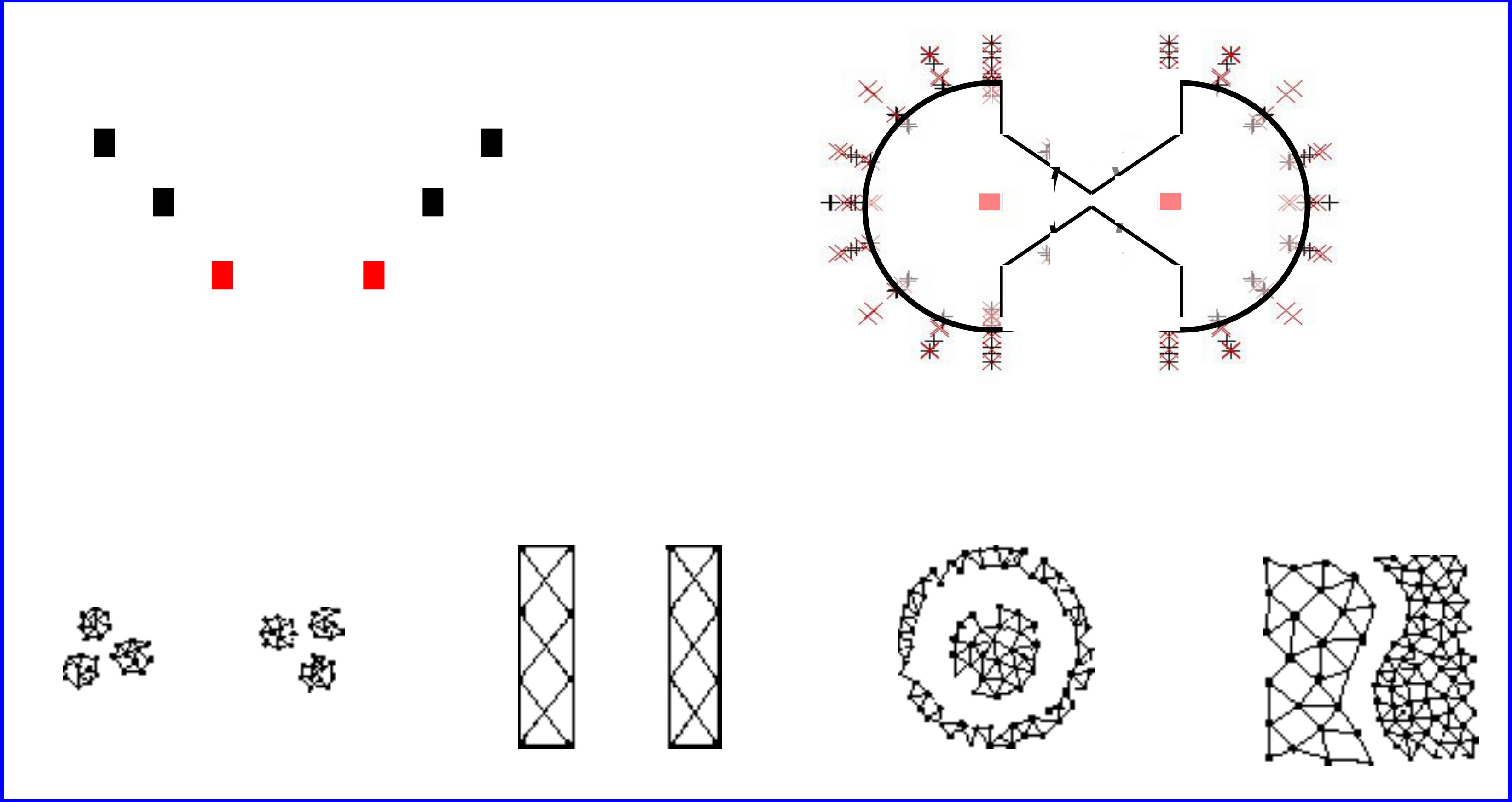


- Clusters are nested
- Often represented as a tree (dendrogram)
- Join/split history and ‘strength’ preserved

Other approaches

- k-means
  - assign points to k groups
  - re-assign to improve objective function
- model-based
  - likelihood/Bayesian; model search/averaging
- density estimation
  - groups = high-density regions
- classification to cluster
- visually motivated methods

Visual Empirical Regions of Influence (VERI)



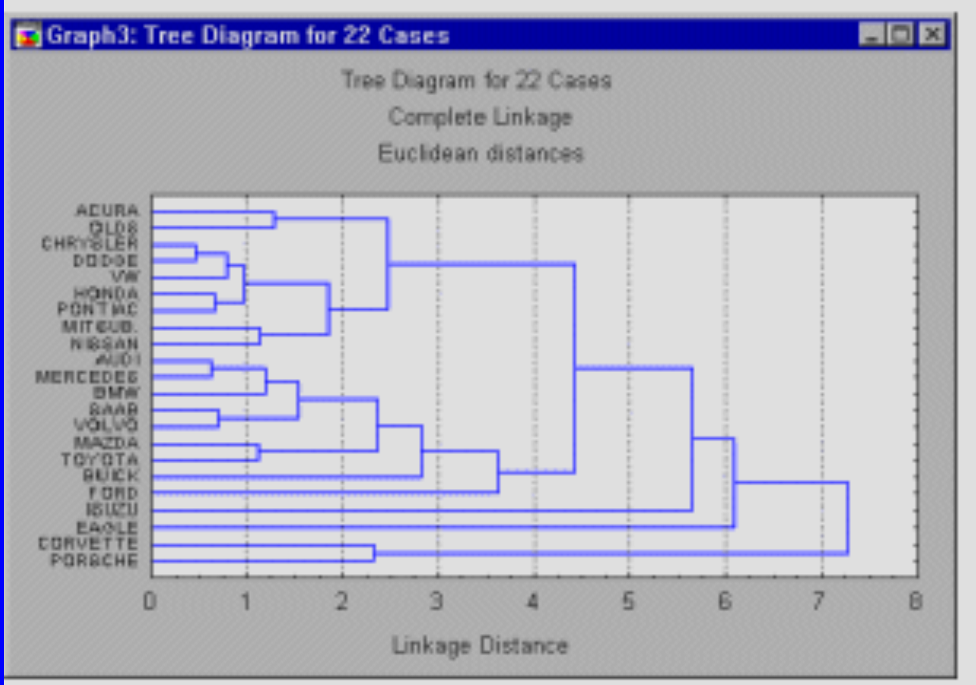
Notes

- many choices
  - between and within methods
- built-in biases for shapes
- computationally costly
  - $O(n^2)$ ...

Conceptual model: algorithmic, run to completion

typical software

- resources dedicated to numerical computation
  - teletype interaction
  - runs to completion
  - graphical “output”



Compare to interactive data analysis

Interactive data analysis

- exploratory, tentative
- graphical
- non-algorithmic
  - varied granularity
- integrated
- deep interaction

3. Enlarging the problem

Mutually exclusive and exhaustive groups

$$g_1, \quad g_2, \quad \ldots, \quad g_k$$

form a partition

$$P = \{g_1, \quad g_2, \quad \ldots, \quad g_k\}$$

of the set of data objects.

Goal: Explore the space of possible partitions.

Structuring the partition space

$P_A=\{g_1, \; g_2, \; \ldots, \; g_a\}$ and $P_B=\{h_1, \; h_2, \; \ldots, \; h_b\}$

- When $a > b$, P_A call a *finer partition* than P_B.
  - P_A is called a *refinement* of P_B (or P_B a *reduction* of P_A)
- P_A is *nested* in P_B only if $a > b$ and *every* g_i is a subset of a single h_j - write $P_A \, \} \, P_B$ or $P_B \, \{ \, P_A$
- When $a = b$, P_A is called a *reassignment* of P_B

Reduction

$P_1=\{g_1, ..., g_6\}$ -> $P_2=\{h_1, \dots, h_4\}$ -> $P_3=\{m_1, m_2, m_3\}$

- $h_i = g_i$ $i = 1, 2$; $h_3 =$ join (g_3, g_4) ; $h_4 =$ join (g_5, g_6)
  - nesting: P_1 } P_2
- disperse elements of h_4 over h_i $i = 1, 2, 3$ to give m_i for $i = 1, 2, 3$.
  - split $(h_4) = \{h_1^*, h_2^*, h_3^*\}$; $m_i =$ join (h_i^*, h_i)
  - P_2 } P_3 is false

Reduction decisions/options

- join operations: which groups?
  - e.g. inner, outer, centres, …
  - distance measures to use …
- dispersal operations:
  - selecting group(s)
    - Max volume, eigen-value, MST…
  - determining partitional method
    - random, VERI, MST, …
  - choosing join …

Refinement

$P_2=\{h_1, \ldots, h_4\}$ ---> $P_1=\{g_1, \ldots, g_6\}$

- $g_i = h_i$ $i = 1, 2$; split (h_3) -> g_3, g_4

  split (h_4) -> g_5, g_6

nesting: P_2 { P_1

Refinement decisions/options

- which groups to split?
  - e.g. inner, outer, directions, …
  - distance measures to use …
- how to split?
  - MST, outlying points, reassignment, ...

Reassignment

$$P_1=\{g_1, ..., g_k\} \text{ -> } P_2=\{h_1, \ldots, h_k\}$$

- objective function $d(P)$ to be minimized. P <- P_1
- for each object o in g_i, assign it to one of g_j (j != i) forming a new partition P_{ij} and find largest

$$\Delta_{ij}(o) = d(P) - d(P_{ij})$$

- repeat for all i, j. If $\max \Delta_{ij} > 0$ move o from g_i, to g_j
- Repeat until $\Delta_{\max} <= 0$

Reassignment decisions/options

- Objective function
  - distances, centres, …
  - within vs between/within, ...
  - variates/directions
- Iteration strategy
  - single-pass, k-means, complete looping (greedy), start, …

4. Putting it together

Series of moves in partition space:

1. Refine (P) -- > P_{new}

2. Reduce (P) -- > P_{new}

3. Reassign (P) -- > P_{new}

Additional ops on partitions

- Unary:
  - Subset (P)
  - Operate any of R (subset (P))
  - Manual (P) … change P according to manual intervention (e.g. colouring)

n-ary operators

- resolve (P_1, ..., P_m) --> P_{new}
- dissimilarity (P_i, P_j) --> $d_{i,j}$
- display (P_1, ..., P_m)
  - dendrogram if P_1 { …{ P_m
  - mds plot of all clusters in P_1, …, P_m
  - mds plot of all partitions P_1, …, P_m

5. Software modelling

- Principal control panel:
  - current partition and list of saved partitions
  - refine, reduce, re-assign, re-start buttons
  - cluster plot button (mds plot)
  - random select button
  - subset focus and join toggle
  - operation on partitions button
  - manual button (form partition from point colours)

Secondary panels

- Refine:
  - performs refine, offers access to arguments
- Reduce
  - performs reduce, offers access to arguments
- Reassign
  - performs reassign, offers access to arguments
- Each will operate on only those points highlighted or on all if none selected.

Secondary panels (continued)

- Operate on partitions
  - saved partitions list
  - resolve selected partition
  - plot selected partitions using selected dissimilarity
  - dendrogram of selected partitions (if nested)
  - cluster-plot for clusters of selected parttitions (esp. for non-nested)

Software modelling (details)

- Objects:
  - Point-symbols, case-objects (existing in Quail)
  - Cluster-points
  - Clusters
  - Partitions
- Methods
  - Reduce, refine, reassign, ...

Software illustration

- Two prototype displays (buggy)
  - Single-window
  - Separate windows
- Integration with existing Quail graphics
- Manual, dendrogram, cluster plots, …
- VERI clustering

6. Summary

- Cluster analysis is naturally exploratory and needs integration with modern interactive data analysis.
- Enlarging the problem to partitions:
  - simplifies and gives structure
  - encourages exploratory approach
  - integrates naturally
  - introduces new possibilities (analysis and research)

Acknowledgements

- Erin McLeish, several undergraduates and graduate students in statistical computing course at Waterloo
- Quail: Quantitative Analysis in Lisp

  http:/www.stats.uwaterloo.ca/Quail