Dissimilarity Plots
A Visual Exploration Tool for Partitional Clustering

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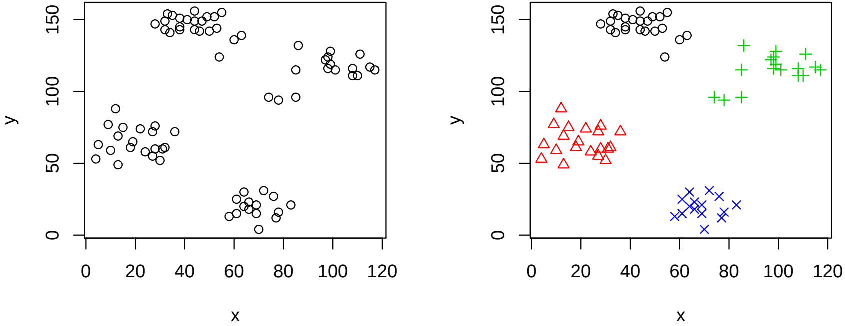
Cluster Analysis

Clustering assigns objects to groups (clusters) so that objects from the same cluster are more similar to each other than to objects from other clusters.

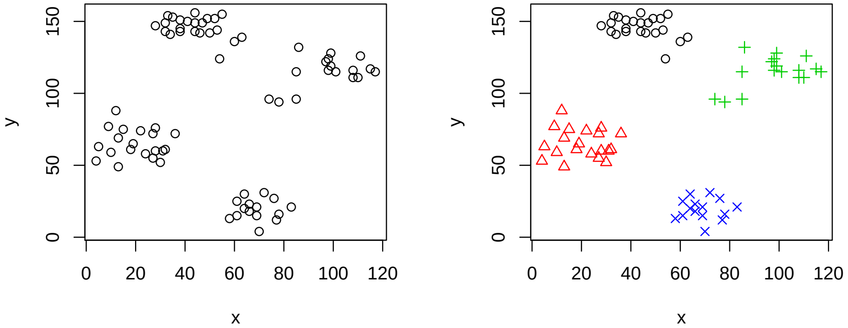


Applications

- Unsupervised learning of structure in the data and summarizing data.
- Areas: Business (market segmentation), biology (communities), social networks, AI, etc.

Assessment of Cluster Quality

Clustering assigns objects to groups (clusters) so that objects from the same cluster are more similar to each other than to objects from other clusters.

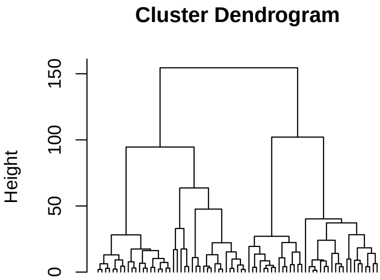


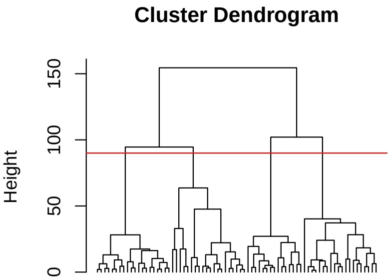
Assess the quality of a cluster solution

- Typically judged by intra and inter-cluster similarities
- Visualization for judging the quality of a clustering and to explore the cluster structure

Dendrograms

Dendrograms (Hartigan, 1967) for hierarchical clustering:





Restriction

Dendrograms are only possible for hierarchical/nested clusterings.

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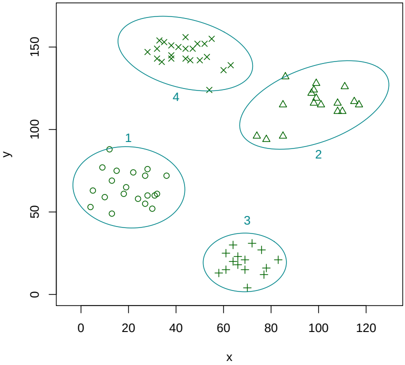
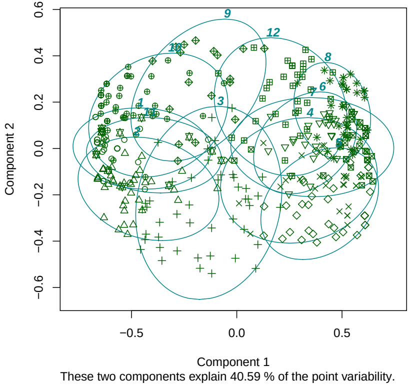
Project objects into 2-dimensional space with dimensionality reduction techniques (e.g., PCA, MDS; Pison *et al.* (1999)).

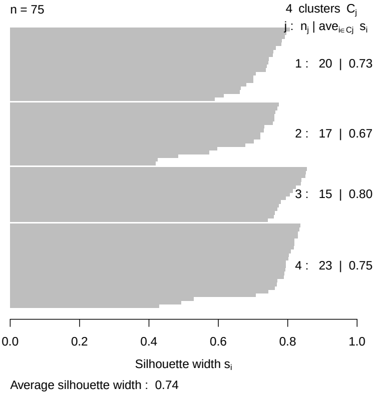




Problems with dimensionality (figure to the right: MDS/32-dimensional data)

Plot Quality Metrics

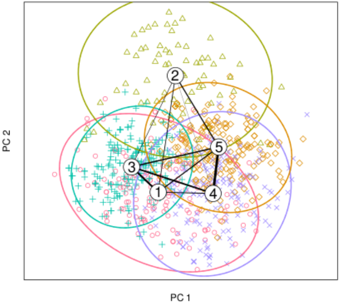
Visualize metrics calculated from inter and intra-cluster similarities to judge cluster quality. For example, **silhouette width** (Kaufman and Rousseeuw, 1990).



→ Only a diagnostic tool for cluster quality

Other Visualization Methods

Several other visualization methods (e.g., based on self-organizing maps and neighborhood graphs, shadow plots, shadow-stars, stripes plots) are reviewed and introduced in Leisch (2008, 2010).



Neighborhood graph

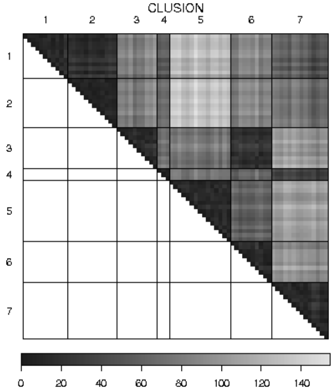
- Typically hide structure within clusters or
- are limited by the number of clusters and dimensionality of data.

Dissimilarity Matrix Shading and CLUSION

Each cell of the (dissimilarity) matrix is represented by a gray value (Sneath and Sokal, 1973; Ling, 1973; Gale *et al.*, 1984). Initially matrix shading was used with hierarchical clustering → **heatmaps**.

For graph-based partitional clustering: **CLUSION** (Strehl and Ghosh, 2003).

Uses **coarse seriation** such that "good" clusters from blocks around the main diagonal.



CLUSION allows to judge cluster quality but does not reveal the structure of the data

→ Dissimilarity plots

Improve matrix shading/CLUSION with (near) optimal placement of clusters and objects within clusters using **seriation**

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Seriation I

Part of **combinatorial data analysis** (Arabie and Hubert, 1996)

- **Aim:** arrange objects in a linear order given available data and some loss function in order to reveal structural information.
- **Problem:** Requires to solve a discrete optimization problem
  $\rightarrow$ solution space grows by the order of $O(n!)$

Seriation I

Part of **combinatorial data analysis** (Arabie and Hubert, 1996)

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Techniques:

1. Partial enumeration methods (currently solve problems with $n \leq 40$)
   - dynamic programming (Hubert *et al.*, 1987)
   - branch-and-bound (Brusco and Stahl, 2005)
2. Heuristics for larger problems

Seriation II

- Set of n objects $\mathcal{O} = \{O_1, O_2, \ldots, O_n\}$.
- Symmetric dissimilarity matrix $\mathbf{D} = \{d_{ij}\}$, where d_{ij} for $1 \leq i, j \leq n$ represents the dissimilarity between O_i and O_j, and $d_{ii} = 0$ for all i.
- Permutation function $\psi_\pi(\mathbf{D}) = \{d_{\pi(i),\pi(j)}\} = \mathbf{P}_\pi \mathbf{D} \mathbf{P}_\pi^T$ reorders the objects in $\mathbf{D}$ by simultaneously permuting rows and columns according to a permutation π. $(\mathbf{P}_\pi = \psi_\pi(\mathbf{I}_n))$
- A loss function L to evaluate a given permutation.

$\mathbf{D}$

	O_3	O_2	O_1	O_4
O_3	0	4	1	8
O_2	4	0	2	2
O_1	1	2	0	3
O_4	8	2	3	0

$\pi = \{3, 2, 1, 4\}$

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Optimization problem

$$\text{minimize } Z = L(\psi_\pi(\mathbf{D}))$$
$$\text{s.t.} \quad \psi_\pi \in \Psi \text{ (valid perm)}$$

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$$\mathbf{D}$$

$$\begin{array}{c|cccc} & O_3 & O_2 & O_1 & O_4 \\ \hline O_3 & 0 & 4 & 1 & 8 \\ O_2 & 4 & 0 & 2 & 2 \\ O_1 & 1 & 2 & 0 & 3 \\ O_4 & 8 & 2 & 3 & 0 \end{array}$$

$\pi = \{3, 2, 1, 4\}$

Optimization problem

$$\text{minimize } Z = L(\psi_\pi(\mathbf{D}))$$
$$\text{s.t.} \quad \psi_\pi \in \Psi \text{ (valid perm)}$$

How should the loss function be defined?

Column/Row Gradient Measures I

Perfect anti-Robinson matrix (Robinson, 1951): A symmetric matrix where the values in all rows and columns only increase when moving away from the main diagonal. Gradient conditions (Hubert *et al.*, 1987):

$$\begin{array}{rlll} \text{within rows:} & d_{ik} \leq d_{ij} & \text{for} & 1 \leq i < k < j \leq n; \\ \text{within columns:} & d_{kj} \leq d_{ij} & \text{for} & 1 \leq i < k < j \leq n. \end{array}$$

$$\mathbf{D} \quad \begin{array}{c|cccc} & O_1 & O_2 & O_3 & O_4 \\ \hline O_1 & 0 & 4 & 1 & 8 \\ O_2 & 4 & 0 & 2 & 2 \\ O_3 & 1 & 2 & 0 & 3 \\ O_4 & 8 & 2 & 3 & 0 \end{array} \qquad \mathbf{\Psi(D)} \quad \begin{array}{c|cccc} & O_1 & O_3 & O_2 & O_4 \\ \hline O_1 & 0 & 1 & 4 & 8 \\ O_3 & 1 & 0 & 2 & 3 \\ O_2 & 4 & 2 & 0 & 2 \\ O_4 & 8 & 3 & 2 & 0 \end{array}$$

Moves similar items (O_1 and O_3) closer together.

Note: Most matrices can only be brought into a near anti-Robinson form.

Column/Row Gradient Measures II

Loss measure (quantifies the divergence from anti-Robinson form):

$$L(\mathbf{D}) = \sum_{i<k<j} f(d_{ik}, d_{ij}) + \sum_{i<k<j} f(d_{kj}, d_{ij})$$

where $f(\cdot,\cdot)$ is a function which defines how a violation or satisfaction of a gradient condition for an object triple (O_i, O_k and O_j) is counted.

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Raw number: Violations minus satisfactions:

$$f(z, y) = \operatorname{sign}(y - z) = \begin{cases} -1 & \text{if} \quad z > y; \\ 0 & \text{if} \quad z = y; \\ +1 & \text{if} \quad z < y. \end{cases}$$

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Weighted: Weight each satisfaction or violation by its magnitude (absolute difference between the values):

$$f(z, y) = |y - z| \operatorname{sign}(y - z) = y - z$$

Hamiltonian Path Length

- $\mathbf{D}$ is seen as a finite weighted graph $G = (\Omega, E)$ with $\Omega = \{O_1, O_2, \ldots, O_n\}$ and the weight w_{ij} for edge $e_{ij} \in E$ represents d_{ij}.
- An order Ψ can be seen as a **Hamiltonian path** through the graph.
- Minimizing the path length results in a seriation optimal with respect to dissimilarities between neighboring objects (Hubert, 1974; Caraux and Pinloche, 2005).

Loss function:

$$L(\mathbf{D}) = \sum_{i=1}^{n-1} d_{i,i+1}$$

$\mathbf{D}$	O_1	O_2	O_3	O_4
O_1	0	**4**	1	8
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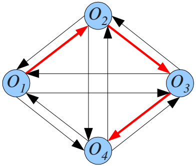

This optimization problem is related to the **traveling salesperson problem** (Gutin and Punnen, 2002) for which good solvers and efficient heuristics exist.

Seriation Criteria

Measure	Definition
Gradient conditions	
Anti-Robinson (AR) events (Chen, 2002)	$\sum_{i<k<j} f(d_{ik}, d_{ij}) + f(d_{kj}, d_{ij})$, with $f(x, y) = I(x > y)$
AR deviations (Chen, 2002)	with $f(x, y) = \lvert y - x\rvert\, I(x > y)$
Gradient measure (Hubert *et al.*, 2001)	with $f(x, y) = -\operatorname{sign}(y - x)$
Weighted gradient measure (Hubert *et al.*, 2001)	with $f(x, y) = -\lvert y - x\rvert \operatorname{sign}(y - x)$
Relative generalized Anti-Robinson events (RGAR) (Tien *et al.*, 2008)	$\frac{1}{m} \sum_{i=1}^{n} \Big(\sum_{(i-w)\le i<k<j} I(d_{ik} < d_{ij}) + \sum_{i<k<j\le(i+w)} I(d_{kj} > d_{ij}) \Big)$, with window size $1 < w < n$ and $m = (^2/_3 - n)w + nw^2 - {}^2/_3\, w^3$
Rank/dissimilarity agreement	
Least squares criterion (Caraux and Pinloche, 2005)	$\sum_{i,j=1}^{n} (d_{ij} - \lvert i - j\rvert)^2$
Inertia criterion (Caraux and Pinloche, 2005)	$-1 \times \sum_{i,j=1}^{n} d_{ij}(i - j)^2$
2-Sum criterion (Barnard *et al.*, 1993)	$\sum_{i,j=1}^{n} \frac{1}{1+d_{ij}} (i - j)^2$
Linear seriation criterion (LS) (Hubert and Schultz, 1976)	$-1 \times \sum_{i,j=1}^{n} d_{ij} \lvert i - j\rvert$
Banded anti-Robinson form (BAR) (Earle and Hurley, 2015)	$\sum_{\lvert i-j\rvert \le b} d_{ij}(b + 1 - \lvert i - j\rvert)$ with band width $1 \le b < n$
Path length	
Hamiltonian path length (PL) (Hubert, 1974; Caraux and Pinloche, 2005)	$\sum_{i=1}^{n-1} d_{i,i+1}$

Table: Popular seriation criteria.

Source: Michael Hahsler. An experimental comparison of seriation methods for one-mode two-way data. **European Journal of Operational Research,** 257:133–143, 2017

Seriation Techiques

Technique	Objective function
Criterion optimization methods	
Integer linear programming (ILP) (Brusco, 2002)	Gradient conditions
Dynamic programming (Hubert *et al.*, 2001)	Gradient conditions
Branch-and-bound (Brusco and Stahl, 2005)	Gradient conditions
Genetic algorithm (Goldberg, 1989; Soltysiak and Jaskulski, 1998)	Various
Simulated annealing (ARSA) (Brusco *et al.*, 2008)	Gradient measure
Spectral seriation (Atkins *et al.*, 1999; Ding and He, 2004; Fogel *et al.*, 2014)	2-Sum criterion
TSP solver (various) (Wilkinson, 1971)	Hamiltonian path length
Quadratic assignment problem heuristic (QAP) (Hubert and Schultz, 1976; Caraux and Pinloche, 2005; Goulermas *et al.*, 2016)	2-Sum criterion, linear seriation, inertia or BAR
Dendrogram methods	
Hierarchical clustering (HC) (Eisen *et al.*, 1998)	Other (depends on linkage)
Gruvaeus and Wainer reordering (GW) (Gruvaeus and Wainer, 1972)	Restricted path length
Optimal leaf ordering reordering (OLO) (Bar-Joseph *et al.*, 2001)	Restricted path length
DendSer reordering (Earle and Hurley, 2015)	Various (restricted)
Other methods	
Multidimensional scaling (MDS) (Kendall, 1971)	Other (stress)
Rank-two ellipse seriation (R2E) (Chen, 2002)	None
Sorting Points Into Neighborhoods (SPIN) (Tsafrir *et al.*, 2005)	Other (energy)
Visual Assessment of Tendency (VAT) (Bezdek and Hathaway, 2002)	Other (MST)

Table: Popular seriation techniques.

Source: Michael Hahsler. An experimental comparison of seriation methods for one-mode two-way data. **European Journal of Operational Research,** 257:133–143, 2017 hahsler:Hahsler2016d

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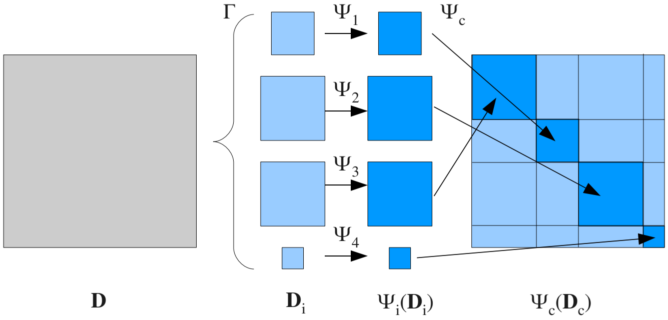
Creating Dissimilarity Plots



1. **Split** $\mathbf{D}$ into clusters using the assignment function Γ provided by the partitional clustering algorithm
2. **Arrange objects:** Use $\Psi_1, \dots, \Psi_k$ to show micro-structure.
3. **Arrange clusters:** Ψ_c places more similar clusters together (macro-structure).

Arrange Clusters

Find Ψ_c based on inter-cluster dissimilarity matrix $\mathbf{D}_c$ which aggregates dissimilarities between all pairs of clusters given dissimilarities between all elements of the clusters in $\mathbf{D}$.

Hierarchical clustering: dissimilarities between two sets of objects $\mathcal{X}$ and $\mathcal{Y}$

$$
\begin{aligned}
\text{complete-link:} \quad & d_c(\mathcal{X},\mathcal{Y}) = \max\{d(x,y) : x \in \mathcal{X}, y \in \mathcal{Y}\} \\
\text{single-link:} \quad & d_s(\mathcal{X},\mathcal{Y}) = \min\{d(x,y) : x \in \mathcal{X}, y \in \mathcal{Y}\} \\
\text{average-link:} \quad & d_a(\mathcal{X},\mathcal{Y}) = \frac{1}{|\mathcal{X}| \cdot |\mathcal{Y}|} \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} d(x,y)
\end{aligned}
$$

Set theory: Hausdorff metric (Hausdorff, 2001)

$$d_H(\mathcal{X},\mathcal{Y}) = \max\{\sup_{x \in \mathcal{X}} \inf_{y \in \mathcal{Y}} d(x,y), \sup_{y \in \mathcal{Y}} \inf_{x \in \mathcal{X}} d(x,y)\}$$

The Hausdorff metric pairs up each element from one set with the most similar element from the other set and then finds the largest dissimilarity in such element pairs.

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Used Seriation Methods

We use the column/row gradient measure as the loss function for seriation.

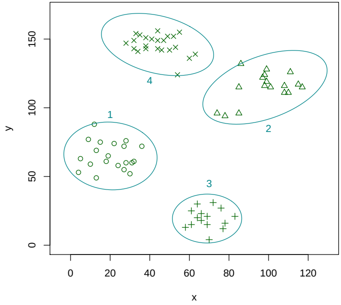
1. Placement (seriation) of clusters: Average-link, row/column gradient measure using branch-and-bound to find the optimal solution
2. Placement (seriation) of objects within each cluster: row/column gradient measure uses a simulated annealing heuristic

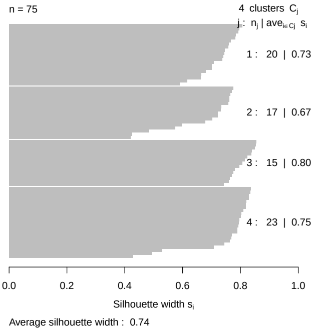
Seriation algorithms are provides by Brusco and Stahl (2005) and are available in the R extension package seriation (Hahsler *et al.*, 2016).

Easily Distinguishable Groups I

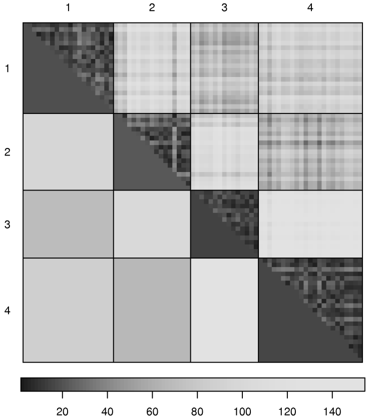
Ruspini data set (Ruspini, 1970) with 75 points in two-dimensional space with four clearly distinguishable groups.

Euclidean distances and k-medoids clustering algorithm (partitioning around medoids (PAM) (Kaufman and Rousseeuw, 1990)) to produce a partition with $k = 4$

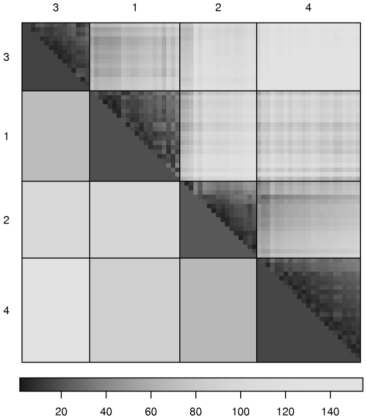




Easily Distinguishable Groups II

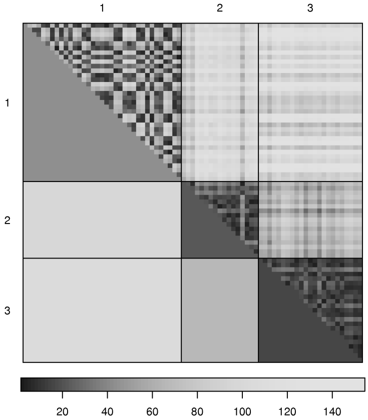


Coarse seriation

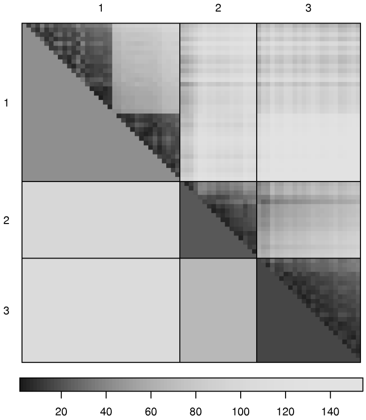


Dissimilarity plot

Mis-specification of the Number of Clusters I

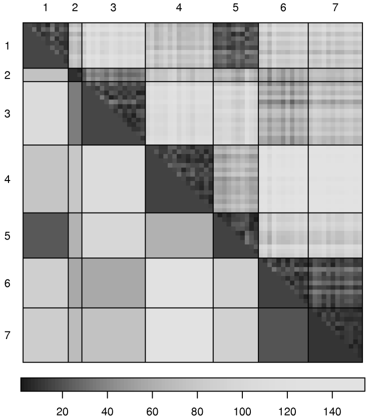


Coarse seriation, $k = 3$

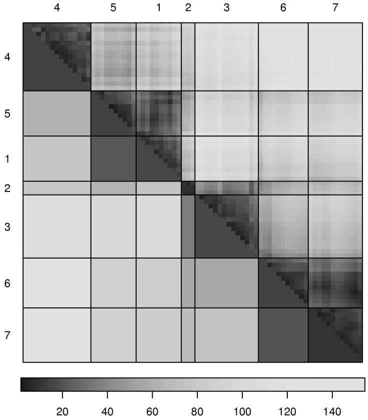


Dissimilarity plot, $k = 3$

Mis-specification of the Number of Clusters II



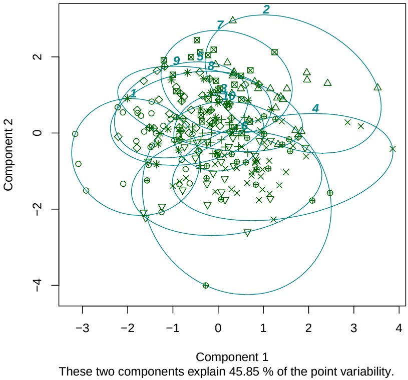
Coarse seriation, $k = 7$

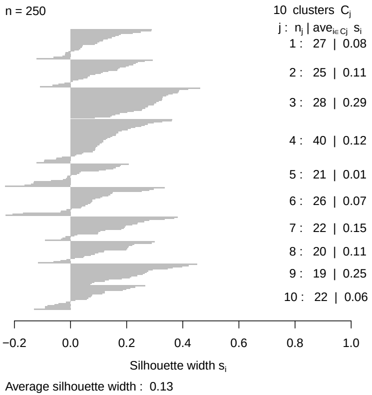


Dissimilarity plot, $k = 7$

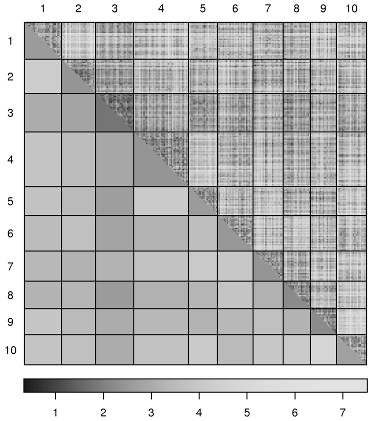
No Structure I

Random data for 250 objects in $\mathbb{R}^5$: $X_1, X_2, \ldots, X_5 \sim N(0,1)$
Euclidean distance and PAM with $k = 10$

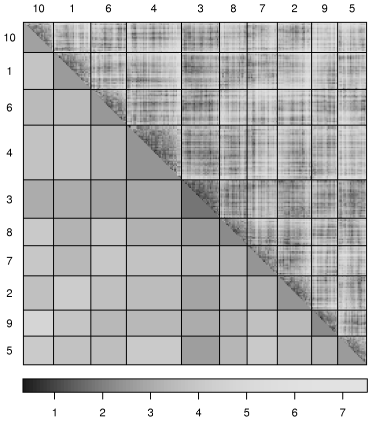




No Structure II



Coarse seriation



Dissimilarity plot

High-dimensional Data I

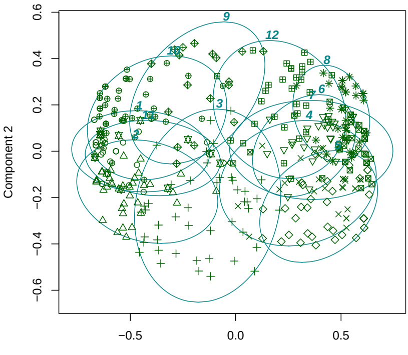
Votes data set (UCI Repository of Machine Learning Databases (Blake and Merz, 1998)). Votes for each of the U.S. House of Representatives congressmen on the 16 key votes during the second session of 1984.

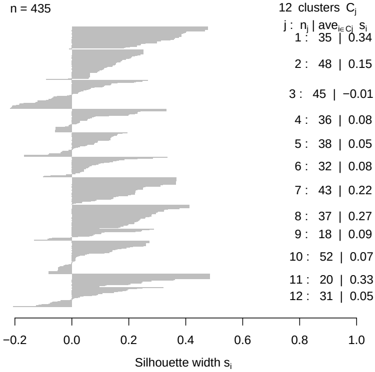
- **Coding:** 2 variables per vote (in favor/agains)
  $\rightarrow$ Each congressman is represented by a vector in $\{0, 1\}^{32}$
- **Dissimilarity measure: Jaccard dissimilarity** (Sneath and Sokal, 1973) between congressmen. Let S_i and S_j be the sets of votes two congressmen cast. Then the Jaccard dissimilarity

$$d_{ij} = 1 - \frac{S_i \cap S_j}{S_i \cup S_j}.$$

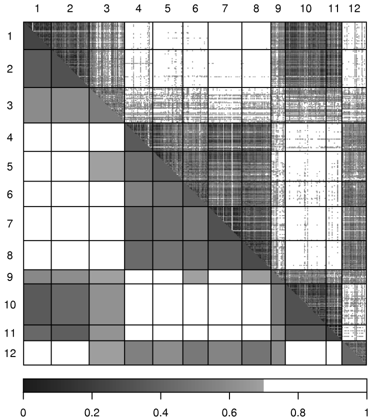
- **Cluster algorithm:** PAM with $k = 12$
  (the first bump of average silhouette for $k = 2, 3, \ldots, 30$)

High-dimensional Data II

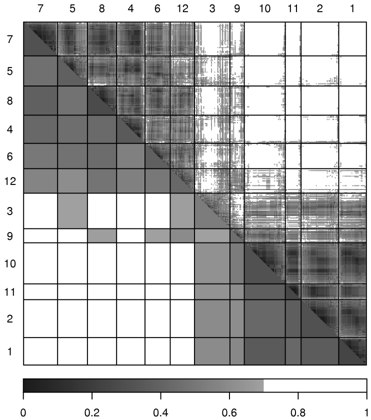




High-dimensional Data III

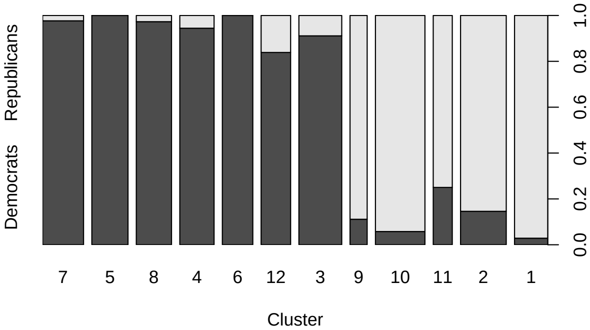


Coarse seriation, threshold=0.7



Dissimilarity plot, threshold=0.7

High-dimensional Data IV



Cluster composition (clusters reordered by dissimilarity plot)

Conclusion

Advantages of dissimilarity plots

- Scales well with dimensionality of data (visualizes dissimilarities)
- Shows cluster quality (block structure)
- Visual analysis of cluster structure (placement of clusters)
- Visual analysis of micro-structure (placement of objects)
- Makes misspecification of number of clusters apparent (placement of clusters/objects)

Enhancements for large number of objects/clusters

- **Object sampling:** Reduces the size of the dissimilarity matrix, however, details are sacrificed.
- **Image downsampling:** pixel skipping, pixel averaging, 2D discrete wavelet transformation
- **Interactive plot:** Plot with only average between-cluster similarities and then separate plot for each cluster (inter-cluster structures).

Further Reading and Code

Further Reading

Michael Hahsler, Kurt Hornik, and Christian Buchta. Getting things in order: An introduction to the R package seriation. **Journal of Statistical Software,** 25(3):1–34, March 2008

Michael Hahsler and Kurt Hornik. Dissimilarity plots: A visual exploration tool for partitional clustering. **Journal of Computational and Graphical Statistics,** 10(2): 335–354, 2011. (Selected for Best of JCGS session 2011)

Michael Hahsler. An experimental comparison of seriation methods for one-mode two-way data. **European Journal of Operational Research,** 257:133–143, 2017.

Code

Dissimilarity plot and seriation methods are implemented in the R extension package seriation (Hahsler *et al.*, 2016) and are freely available via the Comprehensive R Archive Network at

`https://CRAN.R-project.org/package=seriation`.

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