Hierarchical and Pyramidal Clustering for Symbolic Data

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# **Outline**

- Clustering structures
	- −- From the hierarchical to the pyramidal model
- Symbolic Clustering
	- The generalization procedure
	- − $\hbox{--}$  The generality degree
	- − $\hbox{--}$  The clustering algorithm
	- −– The *HIPYR M*odule of SODAS

Hierarchical Model: set of nested partitions

Let S be the observations set (the set being clustered)

Hierarchy on S:Family H on non-empty subsets of S such that

- <sup>S</sup><sup>∈</sup> <sup>H</sup>
- <sup>∀</sup> <sup>s</sup> <sup>∈</sup> S , { s } <sup>∈</sup> <sup>H</sup>
- <sup>∀</sup> h, h' <sup>∈</sup> H, h <sup>∩</sup> h' = Ø or  $h \subseteq h'$  or  $h' \subseteq h$



Pyramidal model:Compatibility between a dissimilarity and an order

S - the observations set (the set being clustered)d - dissimilarity index on S $\theta$  - linear order on S

d and  $θ$  are COMPATIBLE iff, for any ordered triplet,

$$
s_{i} \theta s_{j} \theta s_{k}
$$
\nd(s\_{i}, s\_{k}) \ge Max \{ d(s\_{i}, s\_{j}), d(s\_{j}, s\_{k}) \}

### Pyramid P on S

Family P on non-empty subsets of S such that :

- S ∈ P
- <sup>∀</sup> <sup>s</sup><sup>∈</sup> S , { s } <sup>∈</sup> <sup>P</sup>
- $\bullet$   $\forall$  p, p'  $\in$  P, p  $\cap$  p' = Ø or p  $\cap$  p'  $\in$  P
- There exists a linear order  $\theta$  : every element of P is an interval of  $\theta$

Pyramidal model :





Successor and Predecessor

C – Hierarchy or Pyramid

p ∈ P SUCCESSOR of p'<sup>∈</sup> C if

1) p ⊆ <sup>p</sup>' 2) ¬∃ <sup>p</sup>"∈C : p <sup>⊆</sup> <sup>p</sup>" <sup>⊆</sup> <sup>p</sup>'

p' is a PREDECESSOR of p



Hierarchy : Each cluster has at most ONE predecessor



Pyramid : Each cluster has at most TWO predecessors

### Indexed Hierarchy and Indexed Pyramid

(C, f) with

C – Hierarchy or Pyramid

$$
f: C \rightarrow IR^+
$$
  
a)  $f(h) = 0 \Leftrightarrow \#h = 1$   
b)  $h \subseteq h' \Rightarrow f(h) \le f(h')$ 



Pyramid Indexed in the Broad Sense :

$$
f(p) = f(p')
$$
 with  $p \subset p'$  and  $p \neq p' \Rightarrow$   
 $\exists p_1 \neq p, p_2 \neq p$  such that  $p = p_1 \cap p_2$ 

### Pyramidal (Robinsonian) index

Dissimilarity index d such that :

a) 
$$
d(x, y) = 0 \Rightarrow x = y
$$

b) there exists an order  $\theta$  on S such that

$$
\forall s_i, s_j, s_k \in S, \n s_i \theta s_j \theta s_k \Rightarrow d(s_i, s_k) \ge max \{d(s_i, s_j), d(s_j, s_k)\}
$$

# Pyramidal (Robinsonian) index

d (s<sub>i</sub>, s<sub>j</sub>) = height of the smallest cluster containing s<sub>i</sub> and s<sub>j</sub>

# Johnson-Benzécri Theorem :

Bijection between indexed hierarchies and ultrametricdissimilaritiesHierarchy : d is an ultrametric dissimilarity

# Theorem :<br>Piisetise k

Bijection between pyramids indexed in the broad sense and pyramidal (robinsonian) indices

### Pyramid : d is a pyramidal index The matrix of d ordered according to  $\theta$  is Robinson

### Ascending clustering algorithm

Starting with the one element clusters, merge at each step the MERGEABLE clusters for which the dissimilarity (aggregation index) is MINIMUM

## Mergeable clusters :

- $\bullet$ if the structure is a hierarchy :
- none of them has been aggregated before ;
- $\bullet$ if the structure is a pyramid :
- none of them has been aggregated twice, and
- there is a total order  $\theta$  on S such that the new and all previously formed clusters are intervals of  $\theta$ .

Aggregation Indices :

- Complete Linkage (Maximum Dissimilarity)
- Single Linkage (Minimum Dissimilarity)
- Mean Linkage (Average Dissimilarity)
- Diameter

...

• Ward (Inertia Increase)

**→** Lance & Williams recursive formula; generalized to pyramids



### Abalone data

### Abalone data: Mean linkage pyramid



#### Abalone data:Mean linkage hierarchy



#### Abalone data: Complete linkage pyramid



### Abalone data: Complete linkage pyramid 10% pruned



#### Abalone data: Complete linkage hierarchy



### From classical to symbolic data

 $\textsf{Description:}$  p-tuple  $(\mathsf{d}_1, ..., \mathsf{d}_{\mathsf{p}})$  ,  $\;\mathsf{d}_{\mathsf{j}} \in \mathsf{B}_{\mathsf{j}}$ Description space :  $B = B_1 \times ... \times B_p$ 

Example:

([1000 ,15000] , {drinks (1/4), food (1/2), clothing (1/4)} ,

{Electron, Visa, Mastercard})

Let  $S = \{s_1, \ldots, s_n\}$  the observed set

Then  $:$  Y $_j({\sf s}_i)\in {\sf B}_j$  j=1, $\dots$ , p, i=1, $\dots$ , n

The data array consists on n descriptions, one for each  $\mathsf{s}_\mathsf{i}\in\mathsf{S}\mathsf{:}$ 

$$
(Y_1(s_i), ..., Y_p(s_i))
$$
, i=1,..., n

### Extent and Intent

Extent of a description  $d = (d_1, ..., d_p) \in B$ , Ext (d) : the set of elements  $s \in S$  for which Y $_{\rm j}$  (s) verifies d $_{\rm j}$  , j=1,..., p

 $\mathsf{Internet}\; \mathsf{of}\; \mathsf{a}\; \mathsf{subset}\; \mathsf{C}\subseteq \mathsf{S}$  ,  $\mathsf{Int}(\mathsf{C})$  : the description d = (d<sub>1</sub>, …, d<sub>p</sub>)  $\in$  B such that  $\mathsf{d}_{\mathsf{j}}$  is the minimal element in  $\mathsf{B}_{\mathsf{j}}\,$  (j=1,..., p) fulfilling the condition Y<sub>j</sub> (s) verifies d<sub>j</sub> ∀s∈C

### Example :



d = ( [ 20 , 45]] , [1000 , 4000] ) Ext(d)= { s ∈ S : age(s) <sup>⊆</sup> [ 20 , 45]] <sup>∧</sup> salary(s) <sup>⊆</sup> [1000 , 4000] } Ext (d) = { s1, s<sup>2</sup> , s<sup>3</sup> }



A concept is a pair (C, d) such that

- C is a subset of S
- d is a description,  $d \in B$
- d is the intent of  $C$  :  $Int(C) = d$
- C is the extent of d in E:  $Ext_S(d) = C$

### Example :



Int ({ s<sup>1</sup>, s2 , s3 }) = d = ( [ 20 , 45] , [1000 , 4000] )Ext (d) = { s<sup>1</sup>, s2,, s3 } Int (Ext (d)) = d({ s1, s<sup>2</sup> , s<sup>3</sup> } , d) is a concept

# Symbolic clustering

Objective :

Given a symbolic data array

build an hierarchical / pyramidal clustering

such that each cluster is a concept, i.e., a pair

EXTENSION - its members<br>INTENSION - its description

Each cluster has an automatic representation in terms of the descriptive variables

## Symbolic clustering

- Conceptual clustering methods require:
- •Generalization Operator

 $\mathsf{C} \subseteq \mathsf{C}'$ 

d' (representing C') is more general than

d (representing C)

•Generality degree measure

### Symbolic clustering: Generalisation

→ For a given Extent operator :<br>d is more general than d' if d is more general than d' if the extent of d contains the extent of d'd' is more specific than <sup>d</sup>

Generalisation of two descriptions d and d' : determining d'' : d'' is more general than both d and d',

 $\mathsf{Ext}\,(\mathsf{d}'')\supseteq \mathsf{Ext}\,(\mathsf{d})$  and  $\mathsf{Ext}\,(\mathsf{d}'')\supseteq \mathsf{Ext}\,(\mathsf{d}')$ 

This procedure differs according to the variable type

### Generalisation: Interval variables

 $\mathsf{Consider}\ \mathsf{Ext}(\mathsf{d}) = \{\ \mathsf{s}\in\mathsf{S}: \mathsf{Y}_{\mathsf{j}}(\mathsf{s}) \subseteq \mathsf{d}_{\mathsf{j}}\}$ 

$$
d_j^{(1)} = [I_1, u_1]
$$
;  $d_j^{(2)} = [I_2, u_2]$ 

 $d_j^{(1)} \cup d_j^{(2)} = [\text{Min } \{I_1, I_2\}, \text{Max } \{u_1, u_2\}]$ 

Example :Y<sub>j</sub> = time (min) needed to go to work  $d_i^{(1)} = [5, 15]$ ;  $d_i^{(2)} = [10, 20]$  $d_j^{(1)} \cup d_j^{(2)} = [5, 20]$ 

# Generalisation:Multi-valued categorical variables

Consider Ext(d) = { s  $\in$  S : Y<sub>j</sub>(s)  $\subseteq$  d<sub>j</sub>]

$$
d_j^{(1)} = V_1
$$
;  $d_j^{(2)} = V_2$ 

$$
d_j^{(1)} \cup d_j^{(2)} = V_1 \cup V_2
$$

Example :

$$
Y_j = \text{jobs of a group of people}
$$
  
 $d_j^{(1)} = \{\text{secretary, teacher}\}; d_j^{(2)} = \{\text{employee}\}$   
 $d_j^{(1)} \cup d_j^{(2)} = \{\text{secretary, teacher, employee}\}$ 

Generalisation: Distribution-valued variables

Two possibilities proposed:

take for each category the Maximum of its frequencies

take for each category the Minimum of its frequencies

Distribution-valued variables:Generalisation by the Maximum $d_j^{(1)} \cup d_j^{(2)} = (c_{j1}(p_{j1}^{(1)}), \dots, c_{jk_i}(p_{k_i}^{(1)})) \cup (c_{j1}(p_{j1}^{(2)}), \dots, c_{jk_i}(p_{jk_i}^{(2)})) =$  $t_{i\ell} = \text{Max } \{p_{i\ell}^{(1)}, p_{i\ell}^{(2)}\}$ with  $=$  (c<sub>j1</sub>(t<sub>j1</sub>), ..., c<sub>jk<sub>i</sub></sub>(t<sub>k<sub>i</sub>))</sub> Example :Y<sub>j</sub> = Type of job (administration (0.3), teaching (0.7), secretary  $(0.0)$ )  $\cup$ (administration (0.2), teaching (0.6) , secretary (0.2) ) $=$  (administration  $(0.3)$ , teaching  $(0.7)$ , secretary  $(0.2)$ )  $\overline{C}$ 

Extent: 
$$
{s_i \in S : p_{j\ell}^{(1)} \leq t_{j\ell}, \ell = 1, ..., k_j}
$$

\n"at most" principle

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Distribution-valued variables:Generalisation by the Minimum $d_j^{(1)} \cup d_j^{(2)} = (c_{j1}(p_{j1}^{(1)}),...,c_{jk_i}(p_{k_i}^{(1)})) \cup (c_{j1}(p_{j1}^{(2)}),...,c_{jk_i}(p_{jk_i}^{(2)})) =$  $= (c_{j1}(r_{j1}),...,c_{jkj}(r_{kj}))$  $r_i = Min \{p_{i\ell}^{(1)}, p_{i\ell}^{(2)}\}$ with Example :Y<sub>j</sub> = Type of job (administration (0.3), teaching (0.7), secretary (0.0))  $\cup$  (administration (0.2), teaching (0.6) , secretary (0.2) )= (administration (0.2), teaching (0.6) , secretary (0.0) )

Extent:"at least" principle

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## Symbolic clustering: the algorithm

Starting with the one-object clusters  $\{s_i\}$ , i = 1,...,n

At each step, form a cluster  $\,$  p  $\,$  union of  $\,$  p $_1$  , p $_2$  $\frac{1}{2}$ represented by d such that

- $p_1$ ,  $p_2$  can be merged together
- d is more general than  $d_1$ ,  $d_2$  :  $d = d_1 \cup d_2$ <br>a list  $(a)$
- Int  $(p) = d$
- $Ext_E(d) = p$

Non - uniqueness ⇒ numerical criterion<br>Clusters with rease specific descriptions

 $\rightarrow$  Clusters with more specific descriptions are formed first

## Symbolic clustering: Generality degree

$$
d=(d_1,\ldots,d_p)\qquad \ \ O_j\ \ \text{bounded}
$$



Set-valued variables :

Proportion of the description space covered by d

The more possible members of the extent of d , the greater the generality degree of d

Generality degree: Interval-valued variables

$$
G(d_j) = \frac{m(V_j)}{m(O_j)}
$$
  $m(V_j) = max V_j - min V_j$  (range)

#### Example :

Describing groups of people by age and salaryAge ranges from 15 to 60 , salary ranges from 0 to 10000

0,55 $G(d_1) = \frac{45-20}{60-15} = \frac{25}{45} = 0,55$   $G(d_2) = \frac{3000-1000}{10000} = \frac{2000}{10000} = 0,2$ Consider a group described by $d=[[ 20, 45]$ ,  $[1000, 3000]$ ]) =  $(d_1, d_2)$ 

$$
G(d) = 0,55 \times 0,2 = 0,11
$$

## Generality degree: Multi-valued variables

$$
G(d_j) = \frac{m(V_j)}{m(O_j)}
$$
  $m(V_j) = #V_j$  (cardinal)

#### Example:

Describing groups of people from the UE, defined on variables gender and nationality (28)

Consider one group described by :d= ( { M }, {French, English} ) =  $(d_1, d_2)$ 

$$
G(d_1) = \frac{1}{2} = 0.5
$$
  $G(d_2) = \frac{2}{28} = 0.07$ 

 $G(d) = 0, 5 \times 0, 07 = 0, 035$ 

# Generality degree: Distribution-valued variables

$$
d_j = (c_{j1}(p_{j1}),...,c_{jk_j}(p_{jk_j}))
$$

Generalising by the Maximum:

$$
G_1(d_j)=\frac{1}{\sqrt{k_j}}\sum_{\ell=1}^{k_j}\sqrt{p_{j\ell}}
$$

which is the affinity coefficient (Matusita, 1951) between (p $_{1\ \ell },...,p_{\mathsf{k_j}})$  and the uniform distribution

 $\mathsf{G}_1(\mathsf{d})$  is maximum (=1) when  $\mathsf{p}_{\mathsf{j}\ell}$  = 1/k $_\mathsf{j}$ , i=1,...k $_\mathsf{j}$  : <u>uniform</u>



This means that we consider a description the more general the more similar it is to the uniform distribution

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Generality degree: Distribution-valued variables $d_j = (c_{j1}(p_{j1}),...,c_{jk_j}(p_{jk_i}) )$ 

Generalising by the minimum:

$$
G_2(d)=\frac{1}{\sqrt{k_j(k_j-1)}}\sum_{\ell=1}^{k_j}\sqrt{(1-p_{\ell j})}
$$

Again,  $G<sub>2</sub>(d)$  is maximum (=1)

when 
$$
p_{j\ell} = 1/k_j
$$
, i=1,...k : uniform

### Symbolic clustering: the algorithm

Starting with the one-object clusters  $\{s_i\}$ , i = 1,...,n

At each step, form a cluster  $\,$  p  $\,$  union of  $\,$  p $_1$  , p $_2$  $\overline{2}$  , represented by d such that

- $p_1$ ,  $p_2$  can be merged together
- d is more general than  $d_1$ ,  $d_2$  :  $d = d_1 \cup d_2$
- Int  $(p) = d$  and  $Ext_E(d) = p : (p, d)$  is a concept
- G(d) is minimum

### Symbolic clustering: the algorithm

The algorithm builds a hierarchy / pyramid on S :each cluster is associated to a descriptionwhose extent is the cluster itself

$$
CLUSTER \leftrightarrow CONCEPT
$$
  
CLUSTER = (p, d)   
  $p = Ext d, d = Int(p)$ 

#### automatic representation of the clusters

### Example



#### $Y_i$ : Numerical multi-valued variables



 $P_6: (\{s_1, s_2, s_3\} ; (\{1\}, \{1,2\}, \{1,2\}, \{2,3\}) )$  $P_7: (\{s_1, s_2, s_3, s_4\} ; (\{1,2\}, \{1,2\}, \{1,2\}, \{2,3\}) )$ 



# Symbolic pyramid : Cluster description



### Travel agency data



### Travel agency dataSymbolic pyramid





# The HIPYR module of the SODAS software

Objective :

Perform Hierarchical or Pyramidal clustering on a symbolic data set

- $\bullet$  from a dissimilarity matrix $\rightarrow$  numerical clustering
- $\bullet$  directly based on the data set  $\rightarrow$  symbolic clustering: clusters are concepts

# The HIPYR module of the SODAS software



Structure: Hierarchy or Pyramid

Data Source:

- •Dissimilarity Matrix (Numerical Clustering)
- Symbolic objects (Symbolic Clustering)

Aggregation Index:

- • Numerical Clustering: Maximum, Minimum, Average, Diameter
- • Symbolic Clustering: Minimum Generality Minimum Increase in Generality

- Order Variable (optional) : quantitative single variable; to impose an order compatible with the pyramid
- Modal variables generalization :
	- <mark>– Maximum</mark>
	- Minimum
- Use Taxonomies for generalization

(nominal or categorical multi-valued variables) : Y, N

- Select "best" classes : Y, N
- Write induced dissimilarity/generality matrix : Y, N





### Induced dissimilarity/generality matrix

For each pair of elements of S,  $s_i$ ,  $s_{i'}$ 

 $d^*(s_i,s_i')$  = index (height) of the "smallest" class that contains  $\, {\sf s}_{{\sf i}} \,$  and  ${\sf s}_{{\sf i}'} \,$ 

$$
d^*(s_i, s_{i'}) = Min \{f(C), s_i \in C, s_{i'} \in C\}
$$

Evaluation of the obtained indexed hierarchy / pyramid:Comparision between the initial and the induced dissimilarity/generality matrices.

### Evaluation value

- For  $s_i s_j$ , i, j, =1,..., n, d( $s_i$ ,  $s_j$ ) :
- the given dissimilarity matrix (numerical clustering)
- generality degree of s<sub>i</sub>  $\cup$  s<sub>j</sub> (symbolic clustering)

$$
\frac{\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} (d(s_i, s_j) - d^*(s_i, s_j))^2}{\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} d(s_i, s_j)}
$$

### Cluster selection

Identify the most interesting clusters :



A cluster is "interesting" if its variability is smallas compared to its predecessors.Variability indicated by index values f(h).

Compute mean value and standard deviation of height increase values.

A class is selected if the corresponding increase valueis more than 2 stand. dev. over the mean value.

### Cluster selection



# HIPYR Output

- Text file
- Sodas file
- Interactive Graphical Representation (VPYR)

# HIPYR Output

The output listing contains:

- The labels of the individuals
- The labels of the variables
- The description of each node :
	- −− the symbolic object associated to each node<br>− its extent
	- its extent
- Evaluation value
- •Selected clusters, if asked for
- •The induced matrix, if asked for

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### Graphical Representation



A cluster is selected by clicking on it.

Description of the cluster in terms of

- list of chosen variables
- representation by a Zoom Star





HIPYR - VPYR



Pruning the hierarchy or pyramid using the aggregation

heights as a criterion.

Suppressing cluster p if :

f(p')- $-f(p) < \alpha f(S) \land p$  has a single predecessor

Rate of simplification  $\alpha$ chosen by the user,new graphic window with the simplified structure.



### Graphical Representation: Pruning



### Rule Generation

Hierarchy/pyramid built from a symbolic data table: rules may be generated and saved in a specified file

> Fission method :  $d \Rightarrow d_1 \vee d_2$

Fussion method (pyramids only) :  $\mathsf{d}_1$  $_1 \wedge {\sf d}_2 {\Rightarrow} {\sf d}$ 



### Rule Generation



Reduction

Should the user be interested in a particular cluster,he may obtain a window with the structure restricted to<br>... this cluster and its successors.

### Graphical Representation: Reduction

