A Connection Between Cluster Analysis and Formal Concept Analysis

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Background From Jardine and Sibson

Book: Mathematical Taxonomy by N. Jardine and R. Sibson, Wiley, New York, 1971. This got me started.

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Underlying finite set to be classified: E

$\Sigma(E)$ the reflexive symmetric relations on E.

Dissimilarity coefficient (DC) $d : E \times E \longrightarrow \Re_0^+$

- $d(a, b) = d(b, a)$
- $d(a, a) = 0$

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- $d(a, b) \leq \max\{d(a, c), d(b, c)\}$ for all $a, b, c \in E$.

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Numerically stratified clustering (NSC) $Td : \Re_0^+ \longrightarrow \Sigma(E)$ a residual mapping in that

- There is an h such that $Td(h) = E \times E$.
- $Td(\bigwedge h_i) = \bigcap Td(h_i)$.

NSCs and DCs are in one-one correspondence.

In the book a cluster method is viewed as a transformation of a DC to an ultrametric.

An order theoretic approach

All this suggests an order theoretic framework. This was introduced in a 1978 paper

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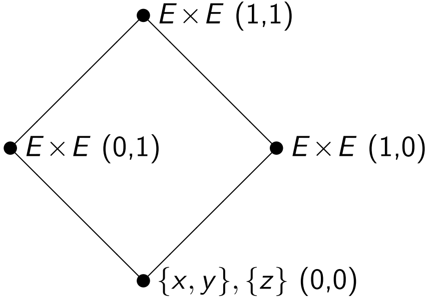
- Thus a DC becomes $d : E \times E \to L$.
- An ultrametric satisfies $d(a, b) \leq d(a, c) \vee d(b, c)$ for all $a, b, c \in E$.
- An NSC remains a residual mapping. This is a well known lattice theoretic mapping and is related to what are called Galois connections.

An Example

Example: $E = \{x, y, z\}$ illustrating the problem.
Dissimilarities measured in 2^2. Here is the input DC

Pairs	Attribute 1	Attribute 2
xy	0	0
xz	1	0
yz	0	1

Cluster Method: Single Linkage Clustering



The levels for cluster $E \times E$ do not occur at a smallest level!

A Modified Model

L is poset with smallest element 0 where dissimilarities measured.

$\mathcal{F}(L) =$ order filters of L ordered by

$F \leq G \iff G \subseteq F$.

$F \neq \emptyset$, $x \in F, x \leq y$ impiles $y \in F$.

Principal filter: $F_h = \{y \in L : y \geq h\}$.

$\mathcal{F}(L)$ is a complete distributive lattice.

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$SD : L \to \Sigma(E)$ (Symmetric relations on E).

Gives cluster candidates at level h.

$SD(h) = \{(a, b) : h \in D(a, b)\}$.

$h \leq k$ implies $SD(h) \subseteq SD(k)$.

If L has a largest member 1, then $SD(1) = E \times E$.

$h \in D(a, b) \iff (a, b) \in SD(h)$.

Boolean Dissimilarities

Assume E has k binary attributes. We want to construct $D : E \times E \to 2^k$, where the ith component of $D(x, y)$ depends only on the values $x(i)$, $y(i)$ of the ith attribute for x and y, If $x(i) \neq y(i)$, we want $D(i) = 1$, so we need only worry about $x(i) = y(i)$.

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(D_1) $D(i) = 0$ if $x(i) = y(i) = 1$ and 1 otherwise

(D_2) $D(i) = 0$ if $x(i) = y(i) = 0$ and 1 otherwise

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For $x = y$, we could either take $D(i) = 0$, or $\bigvee_y \{D(x,y) : x \neq y\}$.

Fact: Each D_i is an ultrametric.

Boolean Dissimilarity Example with $E = \{x, y, z\}$

Objects	A1	A2	A3
x	1	1	0
y	1	0	1
z	0	1	0

D_1	x	y	z
x	001	011	101
y	011	010	111
z	111	111	101

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D_2	x	y	z
x	110	111	110
y	111	101	111
z	110	111	010

D_3	x	y	z
x	000	011	100
y	011	000	111
z	100	111	000

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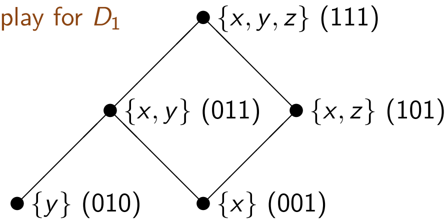
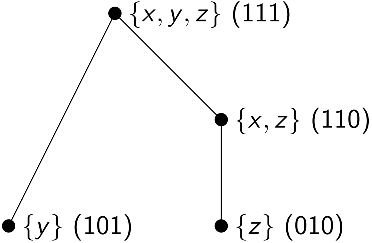
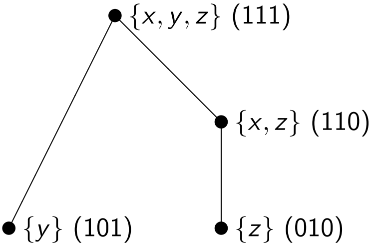
Display for D_1



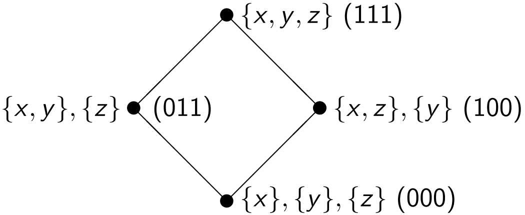
Display for D_2



Display for D_2



Display for D_3



Formal Concept Analysis – thumbnail sketch

Formal Context $\mathfrak{G}, \mathfrak{M}$ sets with

$\perp \subseteq \mathfrak{G} \times \mathfrak{M}$ binary relation called the incidence relation.

Members of $\mathfrak{G}$ objects, $\mathfrak{M}$ attributes.

$A^{\perp} = \{m \in \mathfrak{M} : a \perp m \ \forall a \in A\}$. $B^{\perp} = \{g \in \mathfrak{G} : b \perp g \ \forall b \in B\}$.

$(A \subseteq \mathfrak{G}, B \subseteq \mathfrak{M})$

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$$(A \subseteq \mathfrak{G}, B \subseteq \mathfrak{M})$$

(A, B) formal concept if $A = B^\perp, B = A^\perp$.

Extent is A. *Intent* is B.

For concepts $(A, B), (C, D)$,

$A \subseteq C$ iff $D \subseteq B$.

Order the concepts by inclusion of extents.

Get a complete lattice.

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Nice reference: Introduction to Lattices and Order by Davey and Priestley.

The formal concept approach

Objects	A1	A2	A3
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$\mathfrak{G} = \{x, y, z\}$ $\qquad$ $\mathfrak{M} = \{A1, A2, A3\}$

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$$\{x, y\}^{\perp} = \{A1, A2\} \cap \{A1, A3\} = \{A1\}$$
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$\{y\}^{\perp} = \{A1, A3\}$.

List of formal concepts:

$(\{x, y, z\}, \emptyset)$ $\quad$ $(\{x, y\}, A1)$ $\quad$ $(\{x, z\}, A2)$
$(\{y\}, \{A1, A3\})$ $\quad$ $(\{x\}, \{A1, A2\})$

Comparison of the two approaches

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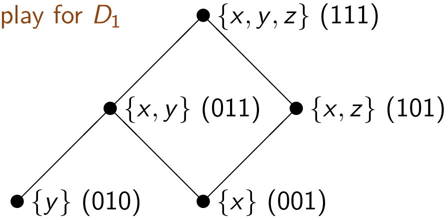

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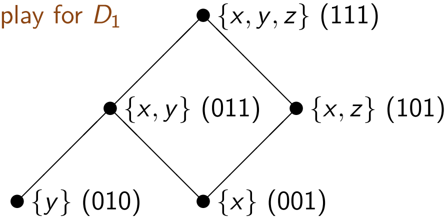
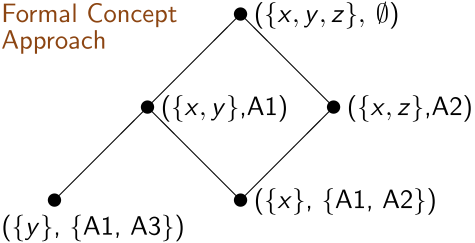


Formal Concept Approach



Complete-Linkage Algorithm

$d : E \times E \rightarrow P$ a poset.

Complete-linkage algorithm:
Assume P is image of d.

1. For each minimal element m, form transitive closure of $Td(m)$. This is output at level m. Call it $F(m)$.
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2. Look at levels h that cover minimal members m
3. For each such h, form $\cup\{F(m) : m < h, m \text{ minimal }\}$. These are all clusters at level h. Add any pairs from $T(h)$. Use complete linkage criterion to merge any clusters.
4. continue the process.

An example involving numerical data

		Water	Protein	Fat	Lactose	Ash
1.	Bison	86.9	4.8	1.7	5.7	0.9
2.	Buffalo	82.1	5.9	7.9	4.7	0.78
3.	Camel	87.7	3.5	3.4	4.8	0.71
4.	Cat	81.6	10.1	6.3	4.4	0.75
5.	Deer	65.9	10.4	19.7	2.6	1.4
6.	Dog	76.3	9.3	9.5	3.0	1.2

Composition of Mammal Milk

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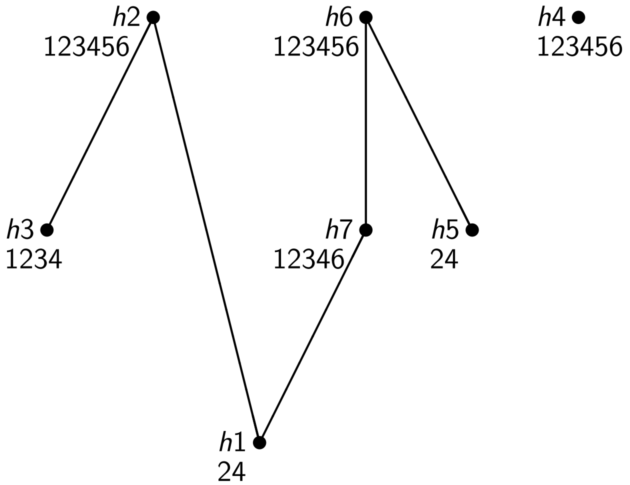
Composition of Mammal Milk

Original data has 25 mammal species. Just wanted a short example. Used dissimilarity taking values in $\mathcal{Z}^5$ where $\mathcal{Z}$ denotes positive integers. Here is construction. Used squared Euclidean distance on each attribute to construct five separate dissimilarities, then represented them as columns in a single dissimilarity matrix having 15 rows and 5 columns. We use the vector ordering inherited from $\mathcal{Z}^5$. To simplify notation, we just rank ordered each column of the matrix. This then produced a dissimilarity taking values in a subposet of $\mathcal{Z}^5$, as displayed in the following table.

Label	object pair	Water	Protein	Fat	Lactose	Ash
$m1$	12	3	3	8	5	4
$m2$	13	2	5	2	4	6
$h1$	14	4	11	6	6	5
$h2$	15	13	12	14	13	12
$h3$	16	9	9	9	12	8
$m3$	23	5	6	5	1	3
$m4$	24	1	8	1	2	1
$h4$	25	12	10	11	10	13
$m5$	26	6	7	1	8	9
$h5$	34	7	14	3	3	2
$h6$	35	14	15	13	11	15
$h7$	36	10	13	7	9	11
$m6$	45	11	1	12	9	14
$m7$	46	4	2	4	7	10
$m8$	56	8	4	10	3	7

Non-minimal Clusters of the Output

For purposes of comparison, standard complete linkage clustering yields the proper clusters 13, 24, 246, 12346.


h2
123456
h6
123456
h4
123456
h3
1234
h7
12346
h5
24
h1
24