A Flexible Metric

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Cees H. Elzinga

PARIS/SILC Research Group Vrije Universiteit Amsterdam

A Joint Enterprise with

- Dr. Matthias Studer, Faculty of Economics and Social Sciences, University of Geneva

- Prof. Hui Wang, Computer Science Research Institute, Ulster University

- Purpose: an SMR-paper on comparing metrics for SA

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Sequence Comparison Methods

- Optimal Matching
  - advantages:
    - well known
    - adaptable edit cost
    - easy algorithm, readily available
  - disadvantages:
    - unequal sequence lengths problematic
    - llcs (OM with unit-cost) crude
- Feature Vectors

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Sequence Comparison Methods

- Optimal Matching
- Feature Vectors
  - advantages:
    - different features possible
    - handles sequences of unequal length
  - disadvantages:
    - generally not well understood
    - “no adaptable edit cost” (Hollister)

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Lecture's Purpose

- Discuss General methodology of feature vectors
- Explain basic algorithm: the Grid
- A flexible representation: weigh for
  - subsequence length
  - subsequence gaps
    - limit gap-size
    - penalize gap-size
  - subsequence characters
  - "edit cost": soft-matching of states
  - durations or run-lengths
- Example(s)

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Sequence Comparison

- To classify
  - sort into groups:
    - that are as different as possible
    - that are as homogeneous as possible
  - collect similar things
    - things that share many features
- To explain (dis)similarity

Simple Sequence Structure

- Sequences are very similar
  - same small alphabet
  - same subsequences e.g. "married - children"
  - same durations e.g. "education"
- Classification is subtle, takes many features

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Feature Vectors: Principles

- select d features or properties $\{p_1, \ldots, p_d\}$
- map each object x to a d-vector $\mathbf{x}$
  - $\mathrm{x} \mapsto \mathbf{x} = (x_1, \ldots, x_d)$
- determine the value of the $\mathbf{x}$-coordinates x_i
  - $$x_i = \begin{cases} f(p_i) & \text{if object } \mathrm{x} \text{ has property } p_i \\ 0 & \text{otherwise} \end{cases}$$
  - simple: $f(p_i) = 1,$ all i (feature "on")

Example: Classifying Beetles

- **Step 1** : Select relevant beetle-properties as vector-coordinates
- **Step 2** : Map different beetles onto different vectors
- **Step 3** : Calculate distances in beetle-space
- **Step 4a**: If beetles are close, put them in the same class
- **Step 4b**: Else, put them in different classes
- **Step 5** : Be happy or try to “explain” the classes

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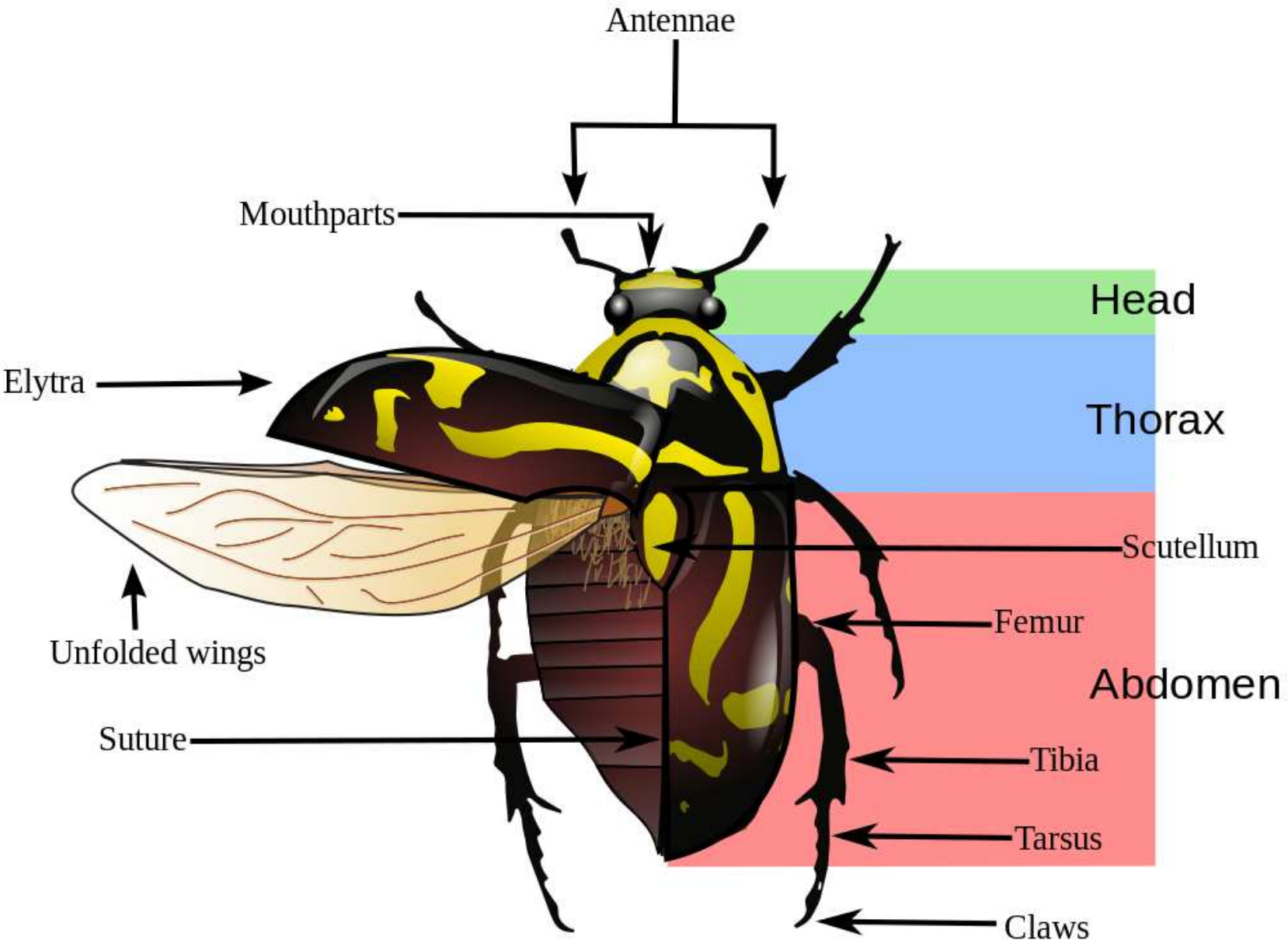
Simple Beetle Morphology



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Many Different Beetles

Binary Beetle Features

Feature	"1"	"0"	discriminates
Long Antennae	yes	no	yes
Compound Eyes	yes	no	yes
Functional Wings	yes	no	yes
6 legs	yes	no	no
Protruding Mouthparts	yes	no	yes
Reads Dickens	yes	no	no
Rowing Legs	yes	no	yes

- 7 binary features suffices to discern $2^7 = 524$ distinct species
- there exist $10^6 - 10^8$ distinct species
  - requires 25-30 binary features

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4 Beetles in Beetle Space $\{0,1\}^7$

Features	$\mathbf{a}$	$\mathbf{b}$	$\mathbf{c}$	$\mathbf{d}$
Antennae	1	0	1	1
Eyes	0	1	0	1
Wings	1	1	0	0
6 legs	1	1	1	1
Mouthparts	1	0	0	1
Reads Dickens	0	0	0	0
Rowing Legs	0	1	0	0

- inner product $\mathbf{a}'\mathbf{b} = \sum_i a_i b_i = 2$ counts common features
- inner product $\mathbf{a}'\mathbf{a} = \sum_i a_i^2 = 5$ counts features

Beetle Feature Vectors

- beetle feature space-matrix $\mathbf{X} = (\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d})$
- Gram-matrix $\mathbf{X}'\mathbf{X} = \begin{pmatrix} 4 & 2 & 2 & 3 \\ 2 & 4 & 1 & 2 \\ 2 & 1 & 2 & 2 \\ 3 & 2 & 2 & 4 \end{pmatrix}$, inner products
- beetle vectors have
  - length: $\|\mathbf{a}\| = \sqrt{\mathbf{a}'\mathbf{a}} = \sqrt{\sum_i a_i^2} = \sqrt{4} = 2$ (“st. dev.”)
  - distance: $d(a, b) = \mathbf{a}'\mathbf{a} + \mathbf{b}'\mathbf{b} - 2\mathbf{a}'\mathbf{b} = 4$
  - angle: $\angle(a, b) = \frac{\mathbf{a}'\mathbf{b}}{\|\mathbf{a}\| \cdot \|\mathbf{b}\|} = \frac{2}{\sqrt{4 \cdot 4}} = 0.5$ (“correlation”)

Careers in Career-Space

- Alphabet $\mathcal{A} = \{a, b, c\}$ (labor market states)
- all strings $\mathcal{A}^*$: set of all possible careers
  - career $\mathrm{x} = abbcaaccbbaaaab\ldots$
  - careers are concatenations of symbols from $\mathcal{A}$
- career features: all sub-careers
  - a, ac, $abacb$, $\ldots$
- map careers onto career-feature vectors

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2 Careers in Career-Space

careers: $\mathrm{x} = abac \mapsto \mathbf{x}$, $\mathrm{y} = bacb \mapsto \mathbf{y}$

subcareers	$\mathbf{x}$	$\mathbf{y}$
a	1	1
$\vdots$	$\vdots$	$\vdots$
aa	1	0
ab	1	1
$\vdots$	$\vdots$	$\vdots$
aba	1	0
$\vdots$	$\vdots$	$\vdots$
acb	0	1
$\vdots$	$\vdots$	$\vdots$

- each possible subsequence is a feature

Feature Vectors: Problems I

- feature selection: relevance?
  - no beetles read Dickens (not applicable)
  - some beetles have horns (not selected)
  - all beetles have 6 legs (non-discriminating)
- feature selection: how many are necessary/acceptable?
  - $\{0,1\}^d$-vectors generate at most 2^d classes
  - dimensionality of subsequence-space is colossal: countably infinite

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Feature Vectors: Problems II

- feature selection: relevance?
- feature selection: how many are necessary/acceptable?
- calculating inner products
  - space/time-consuming because of size
  - “vector-avoiding” algorithms: “Kernels”
- Gram-matrix tends to be orthogonal: big diagonal
  - objects have everything in common with themselves
  - objects have little in common with other objects
  - compress sequences to shorter ones

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Constructing Sequence Vectors

- $\mathcal{A}$: alphabet; $\mathcal{A}^*$: set of all sequences over $\mathcal{A}$
- assign an integer, a rank number $r(u)$ to each $u \in (A)^* = \{u, v, w, \ldots\}$
- define vectors $\mathbf{x} = (\mathrm{x}_1, \mathrm{x}_2, \ldots)$ for each $x \in \mathcal{A}^*$ such that

$$\mathrm{x}_{r(u)} = \begin{cases} f(u,x) & \text{if } u \sqsubseteq x \\ 0 & \text{otherwise} \end{cases}$$

  - $f(u,x)$: "anything we like to use"
    - (as long as we can compute inner products $\mathbf{x}'\mathbf{y}$)
- distance: $d(x,y) = \mathbf{x}'\mathbf{x} + \mathbf{y}'\mathbf{y} - 2\mathbf{x}'\mathbf{y}$
- similarity: $s(x,y) = \mathbf{x}'\mathbf{y}/(\mathbf{x}'\mathbf{x} + \mathbf{y}'\mathbf{y} - \mathbf{x}'\mathbf{y})$

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Constructing Sequence Vectors

$$\mathrm{x}_{r(u)} = \begin{cases} f(u,x) & \text{if } u \sqsubseteq x \\ \\ 0 & \text{otherwise} \end{cases}$$

subsequence weighing	condition	$f(u,x)$
none (commonness)	$u \sqsubseteq x$	1
embedding frequency	$u \sqsubseteq x$	$\lvert x \rvert_u$
length	$u \sqsubseteq x$	$\ell(u)^p, \;\; p > 1$
limit gap-size	$(u \sqsubseteq x) \wedge gaps < d$	any
states	$u \sqsubseteq x$	$\prod_i w(u_i)$
duration	$u \sqsubseteq x$	$\sum_i t(u_i)$
soft-matching any subset sumultaneously	$u \sqsubseteq x$	any, with $\mathbf{x}'\mathbf{y} = \mathbf{x}'\mathbf{S}\mathbf{y}$

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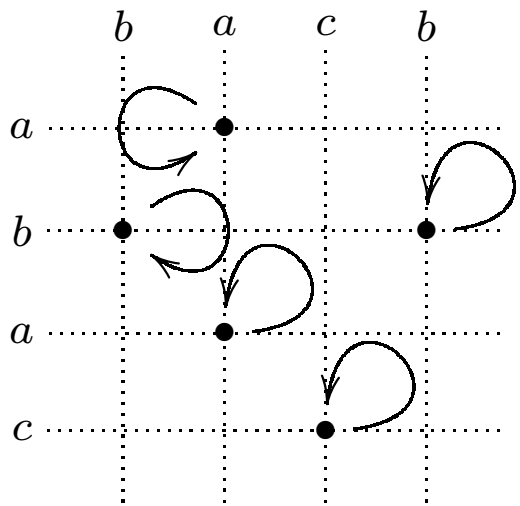
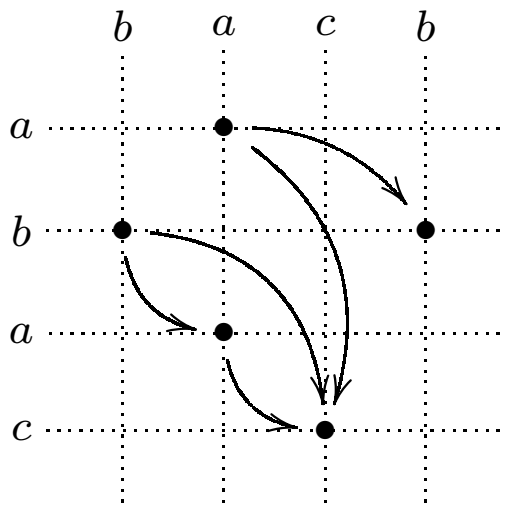
Computations in the Sequence Grid





$$\mathbf{M}^1 = \begin{pmatrix} & 1 & \\ 1 & & 1 \\ & 1 & \\ & & 1 \end{pmatrix} \quad \mathbf{M}^2 = \begin{pmatrix} & 2 & \\ 2 & & 0 \\ & 1 & \\ & & 0 \end{pmatrix} \quad \mathbf{M}^3 = \begin{pmatrix} & 0 & \\ 1 & & 0 \\ & 0 & \\ & & 0 \end{pmatrix}$$

$$\phi_k = \sum_{ij} m_{ij}^k, \quad \mathbf{x}'\mathbf{y} = \sum_k \phi_k = 5 + 5 + 1 = 11$$

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Embedding Frequency

- $x = abac$, $u = ac = x_1x_4 = x_3x_4$, $|x|_u = 2$
- $\mathbf{x}'\mathbf{y}$ counts "matching embeddings": $\sum_u |x|_u \cdot |y|_u$
- when repetition of patterns is important:
  - labor market careers
  - criminal careers
  - animal behavior sequences
- $$\mathrm{x}_{r(u)} = \begin{cases} |x|_u & \text{if } u \sqsubseteq x \\ 0 & \text{otherwise} \end{cases}$$

Length

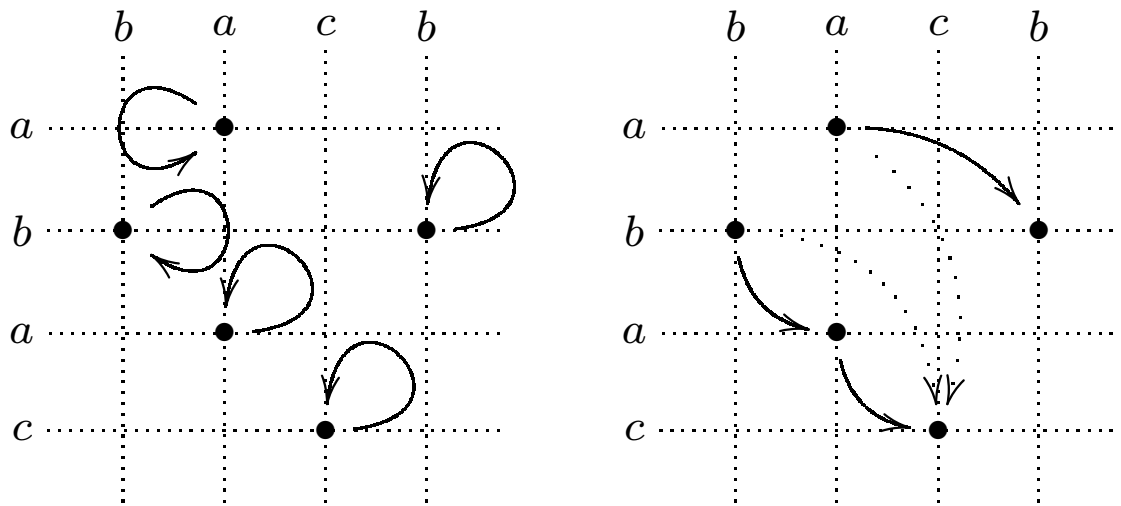
- $x = abac$, $u = ab$, $\ell(u) = 2$
- expect many short common subsequences
- focus on longer subsequences
- OM with standard costing:

$$d(x, y) = \ell(x) + \ell(y) - 2llcs(x, y)$$

- implementation $\mathbf{x}'\mathbf{y} = \sum_k k^p \phi_k$ or more sophisticated

$$\mathrm{x}_{r(u)} = \begin{cases} \ell(u)^p \cdot |x|_u & \text{if } u \sqsubseteq x \\ 0 & \text{otherwise} \end{cases}$$

Limiting the Gap-size



$$\mathbf{M}^1 = \begin{pmatrix} & 1 & & \\ 1 & & & 1 \\ & 1 & & \\ & & 1 & \end{pmatrix} \quad \mathbf{M}^2 = \begin{pmatrix} & 1 & & \\ 1 & & & 0 \\ & 1 & & \\ & & 0 & \end{pmatrix} \quad \mathbf{M}^3 = \begin{pmatrix} & 0 & & \\ 1 & & & 0 \\ & 0 & & \\ & & 0 & \end{pmatrix}$$

$$\phi_k = \sum_{ij} m_{ij}^k, \quad \mathbf{x}'\mathbf{y} = \sum_k \phi_k = 5{+}3{+}1 = 9$$

Weighing States

- some states may be more significant than others
  - unemployed
  - infected
- Assign a weight $w(a_i)$ to each state in $\mathcal{A} = \{a_1, a_2, \ldots\}$
- Calculate the weight of u as $\prod_i w(u_i)$
  - $w(abac) = w(a) \cdot w(b) \cdot w(a) \cdot w(c)$

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Weighing the States

$$x = abac, \quad y = bacb$$

$$w(a) = 2,\ w(b) = 1,\ w(c) = 3$$

$$\mathbf{M}^1 = \begin{pmatrix} & 2 & \\ 1 & & 1 \\ & 2 & \\ & & 3 \end{pmatrix} \quad \mathbf{M}^2 = \begin{pmatrix} & 8 & \\ 6 & & 0 \\ & 6 & \\ & & 0 \end{pmatrix} \quad \mathbf{M}^3 = \begin{pmatrix} & 0 & \\ 6 & & 0 \\ & 0 & \\ & & 0 \end{pmatrix}$$

$$\phi_k = \sum_{ij} m_{ij}^k, \quad \mathbf{x}'\mathbf{y} = \sum_k \phi_k = 9 + 20 + 6 = 35$$

$$\mathrm{x}_{r(u)} = \begin{cases} w(u) \cdot |x|_u & \text{if } u \sqsubseteq x \\ 0 & \text{otherwise} \end{cases}$$

Duration

- $x = x_1 x_2 x_3 \ldots$, $t_x = t_1 t_2 t_3 \ldots$
  - time, pitch, voltage, speed
  - *any* quantifiable state-property
- $t(x) = t_1 + t_2 + t_3 + \ldots$
- $$\mathrm{x}_{r(u)} = \begin{cases} t(u) w(u) \ell(u)^p \cdot |x|_u & \text{if } u \sqsubseteq x \\ 0 & \text{otherwise} \end{cases}$$
- duration is treated like any other weight

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Soft-Matching ("indel cost")

- "Hollister's Problem": some states are more different than others
  - (Single,Married) vs (Cohabitation,Married)
- coordinates are "hard": either 0 or >0
  - $\mathbf{x}'\mathbf{y} = \sum_i x_i y_i$, $x_i = 0$ and/or $y_i = 0 \Rightarrow x_i y_i = 0$
- Inner product compares values of equally indexed coordinates
  - never "compares" subsequences containing "Married" with subsequences containing "Single"
- In OM: substitution cost - compare different states

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Soft-Matching ("indel cost")

- Define state-similarities $\mathbf{M} = (m_{ij})$, $0 \leq m_{ij} \leq 1$, $m_{ii} = 1$, $m_{ij} = m_{ji}$
- calculate $\mathbf{x'My}$ instead of $\mathbf{x'y}$
  - $\mathbf{x'My} = \underbrace{\sum_i x_i y_i}_{\text{"}hard\text{"}} + \underbrace{2 \sum_{i \neq j} x_i \cdot m_{ij} \cdot y_j}_{\text{"}soft\text{"}}$
  - $d(x, y) = \mathbf{x'Mx} + \mathbf{y'My} - \mathbf{2x'My}$
  - Euclidean distance in "elliptical" space
  - implementation in Grid-algorithm: $\mathbf{M}^1 \leftarrow \mathbf{M}$

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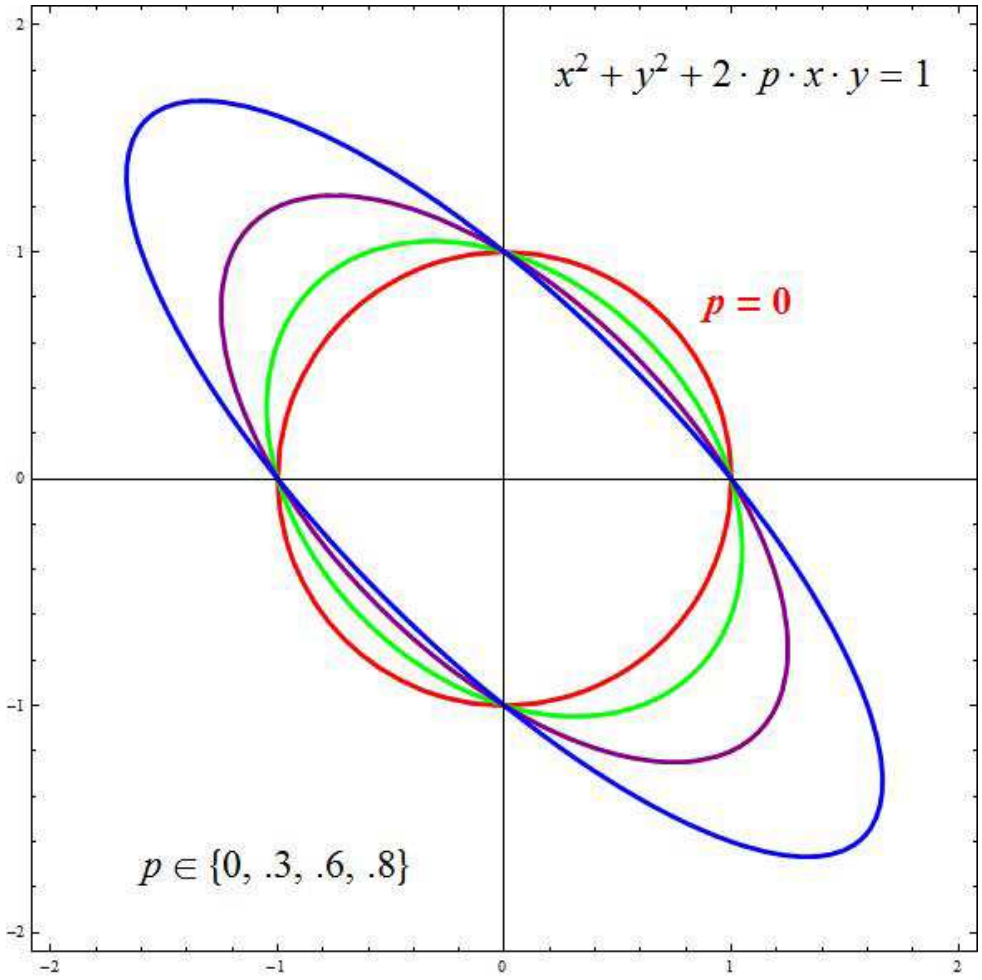
Unit-circles in Elliptical Space



M-Elliptical Circles: $\mathbf{x}'\mathbf{M}\mathbf{x} = 1, \quad \mathbf{M} = \begin{pmatrix} 1 & p \\ p & 1 \end{pmatrix}$

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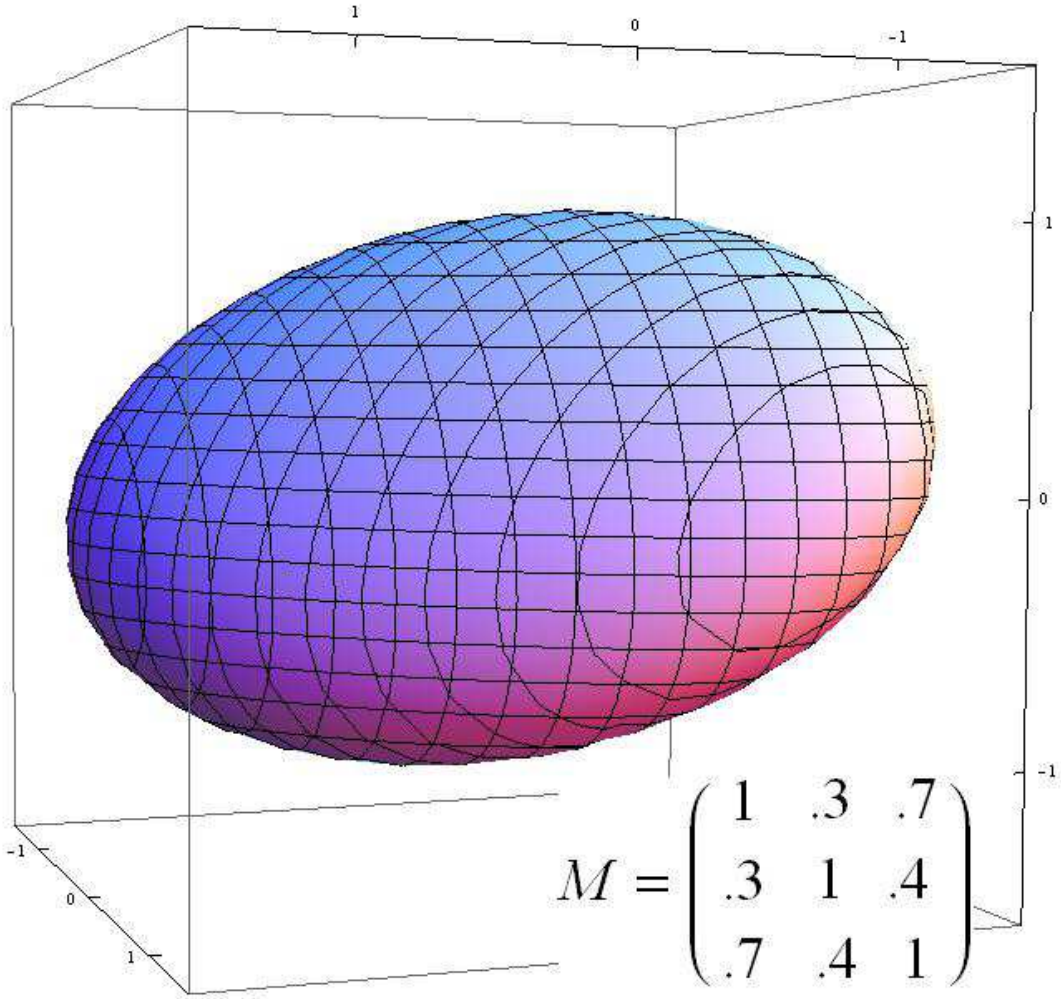
Unit-Sphere in Elliptical Space



$$M = \begin{pmatrix} 1 & .3 & .7 \\ .3 & 1 & .4 \\ .7 & .4 & 1 \end{pmatrix}$$

M-Elliptical 1-sphere

An Application

- Data described in
  - Müller, Gabadinho, Ritschard & Studer: Extracting knowledge from life courses: clustering and visualization, *Data Warehousing and Knowledge Discovery*, Lecture Notes in Computer Science, 2008, Volume 5182/2008, 176-185

- 4318 individuals, born 1909-1972, $\geq$30 years old, retrospective data
  - 4 events: L(eft parental home), (1st) M(arriage), (1st) C(child), (1st) D(ivorce)
  - 8 states: P(no event, still with Parents), L, M, LM, C, LC, LMC, D
  - data example:

birth	L	M	C	D
1974	1992	1994	1996	-

  - sequence example:

74	. . .	91	92	93	94	95	96	97	98	. . .
P	. . .	P	L	L	LM	LM	LMC	LMC	LMC	. . .

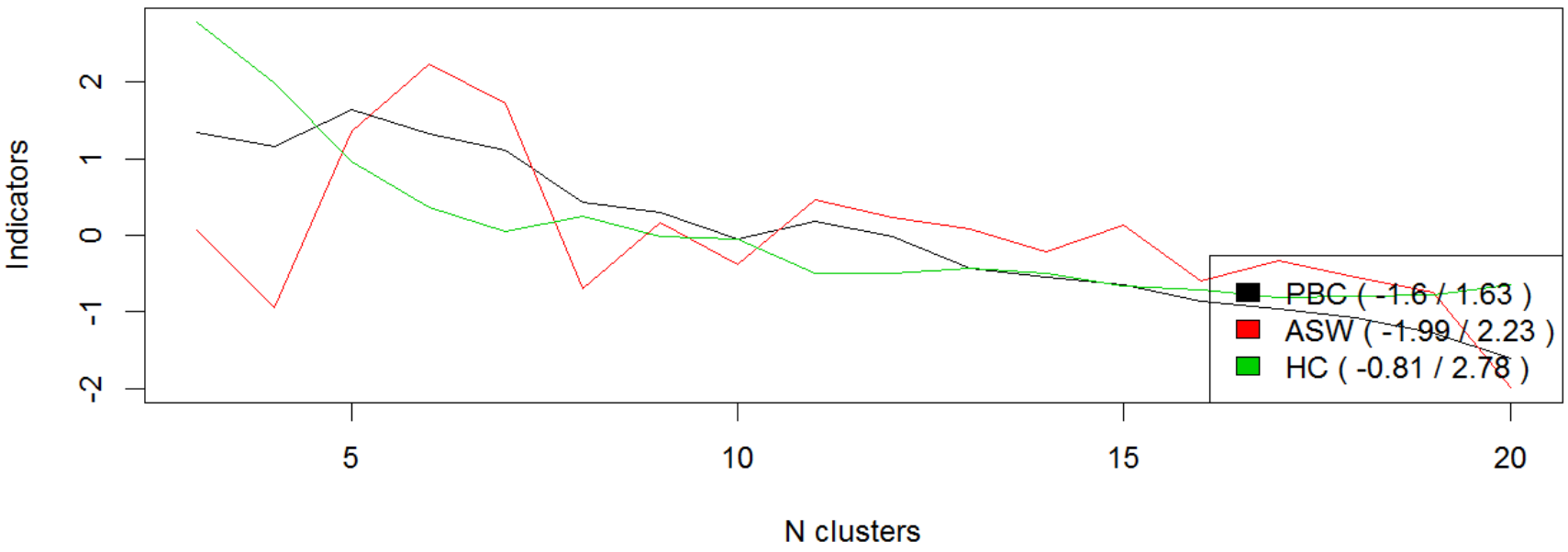
An Application

- OM-cost matrix $\mathbf{C}$:

	P	L	M	LM	C	LC	LMC	D
P	0							
L	.25	0						
M	.38	.62	0					
LM	.50	.25	.38	0				
C	.25	.50	.38	.75	0			
LC	.50	.25	.62	.50	.25	0		
LMC	.75	.50	.38	.25	.50	.25	0	
D	.75	.74	.38	.50	.75	.75	.50	0

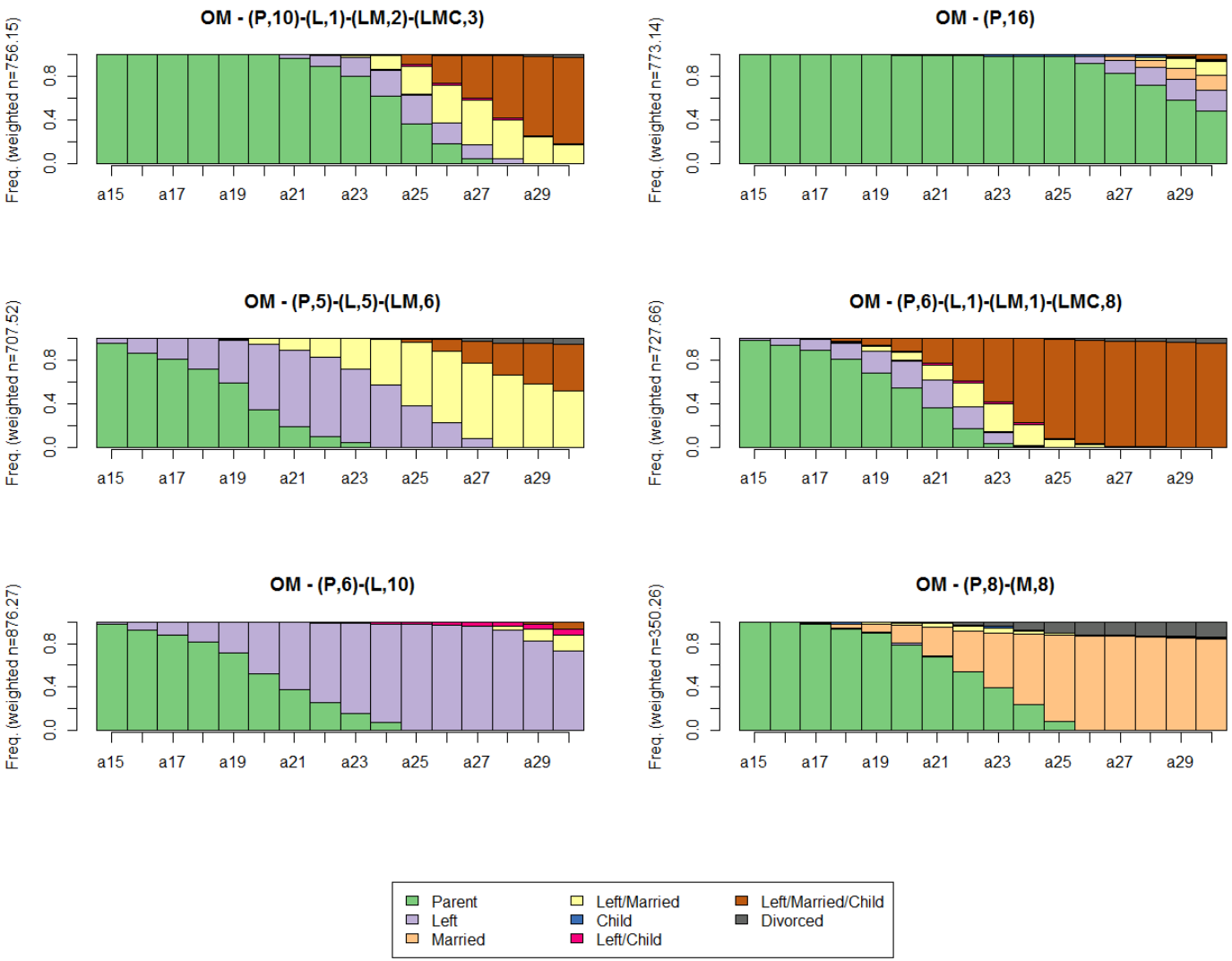
- soft-matching matrix $\mathbf{M} = \mathbf{1} - \mathbf{C}$: $m_{ij} = 1 - c_{ij}$

Finding Clusters (PAM) with d_{OM}

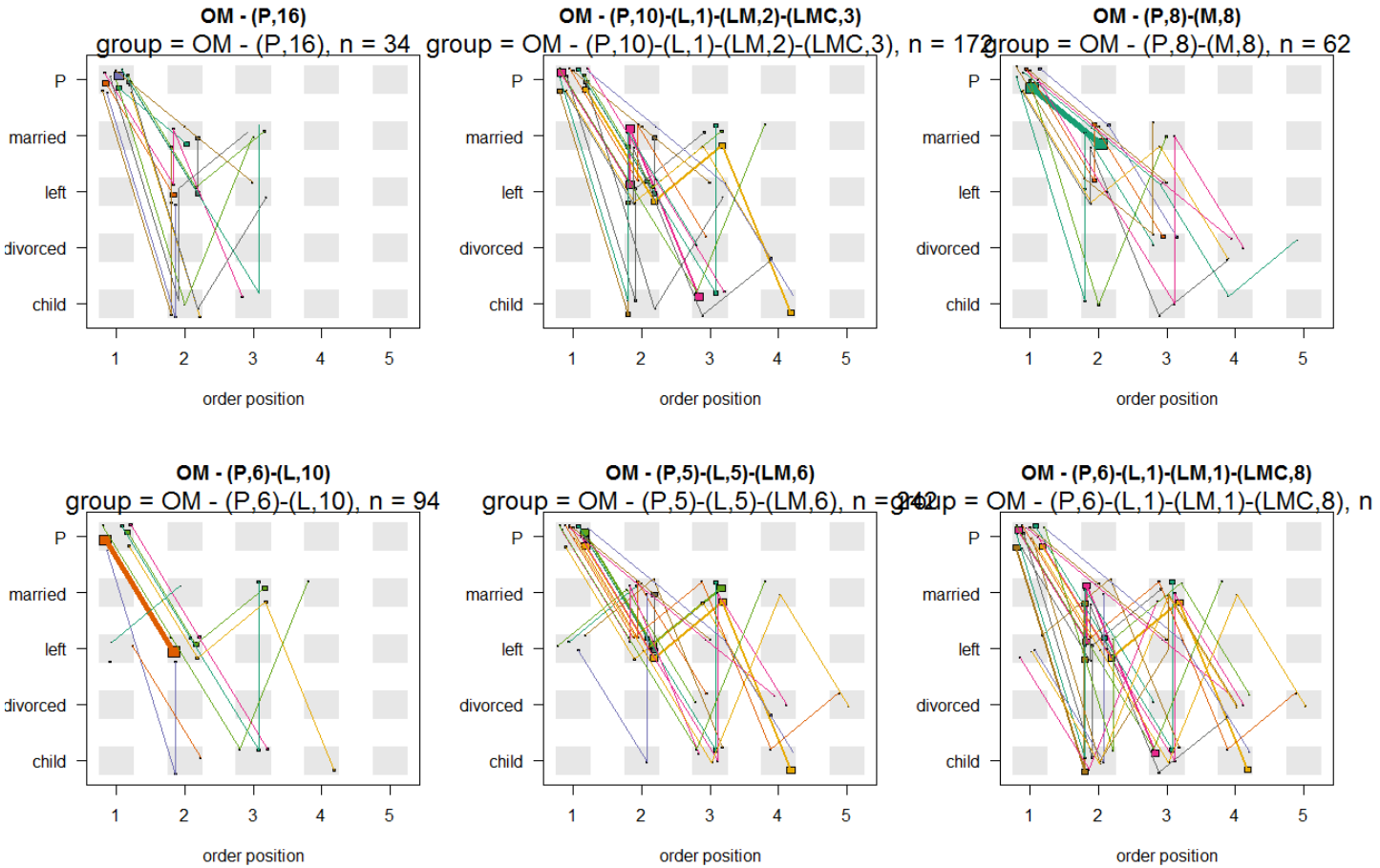


6 clusters seems optimal

OM-cluster profiles: Chronogrammes



OM-cluster profiles: order-plots

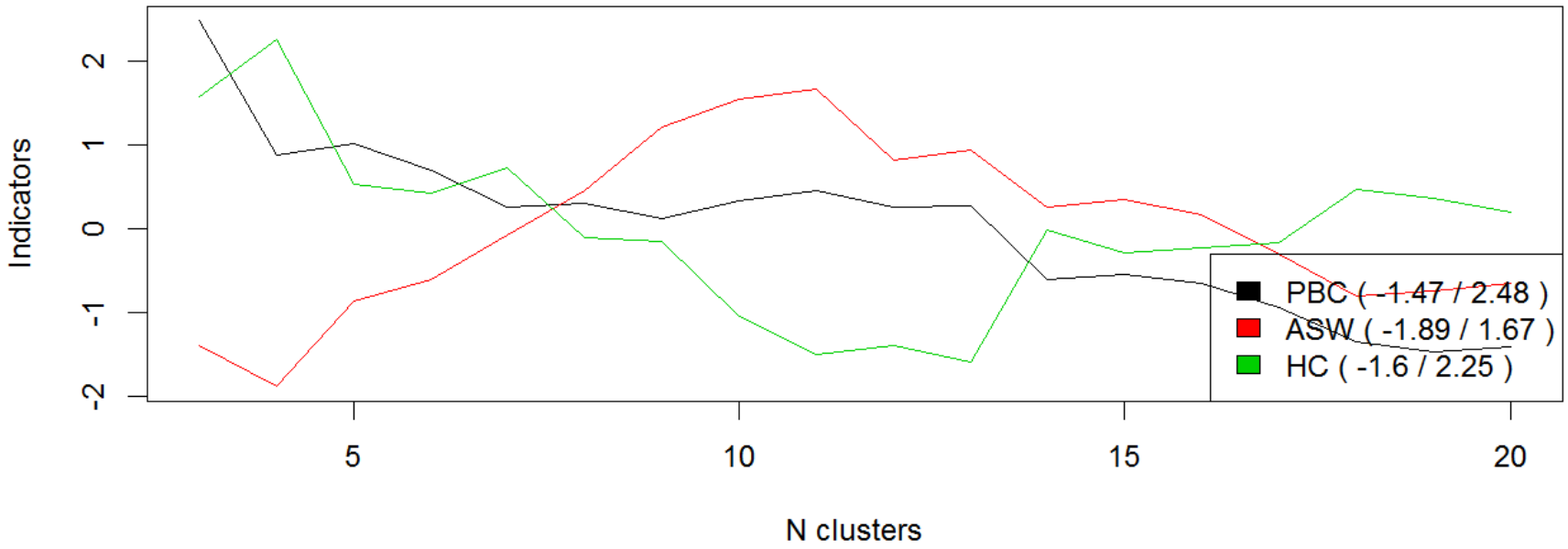


An alternative clustering

Using subsequences, weighed for

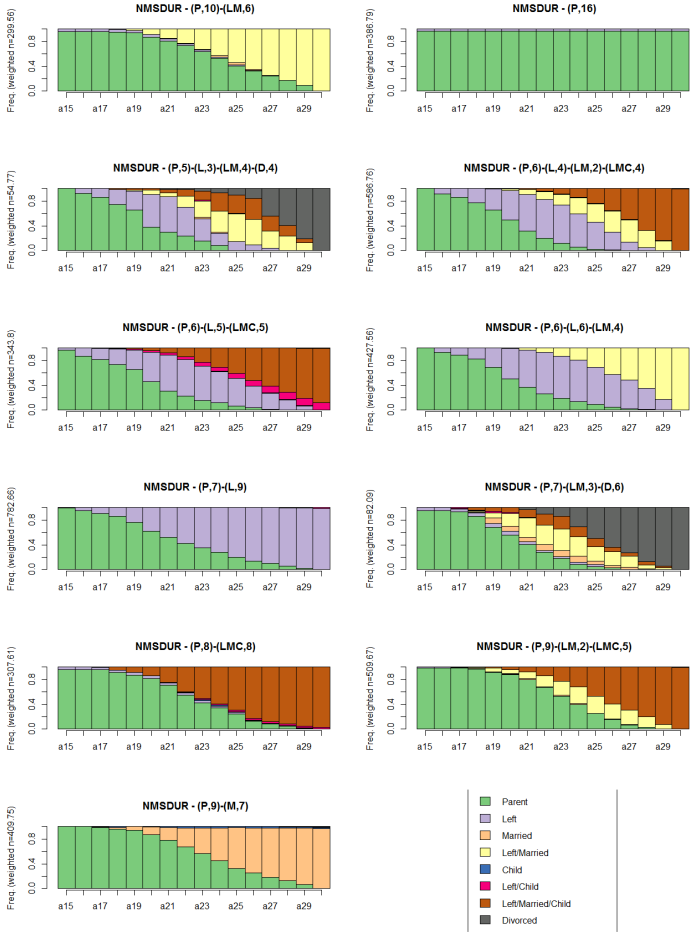
- duration
- embedding frequency

and employing soft-matching

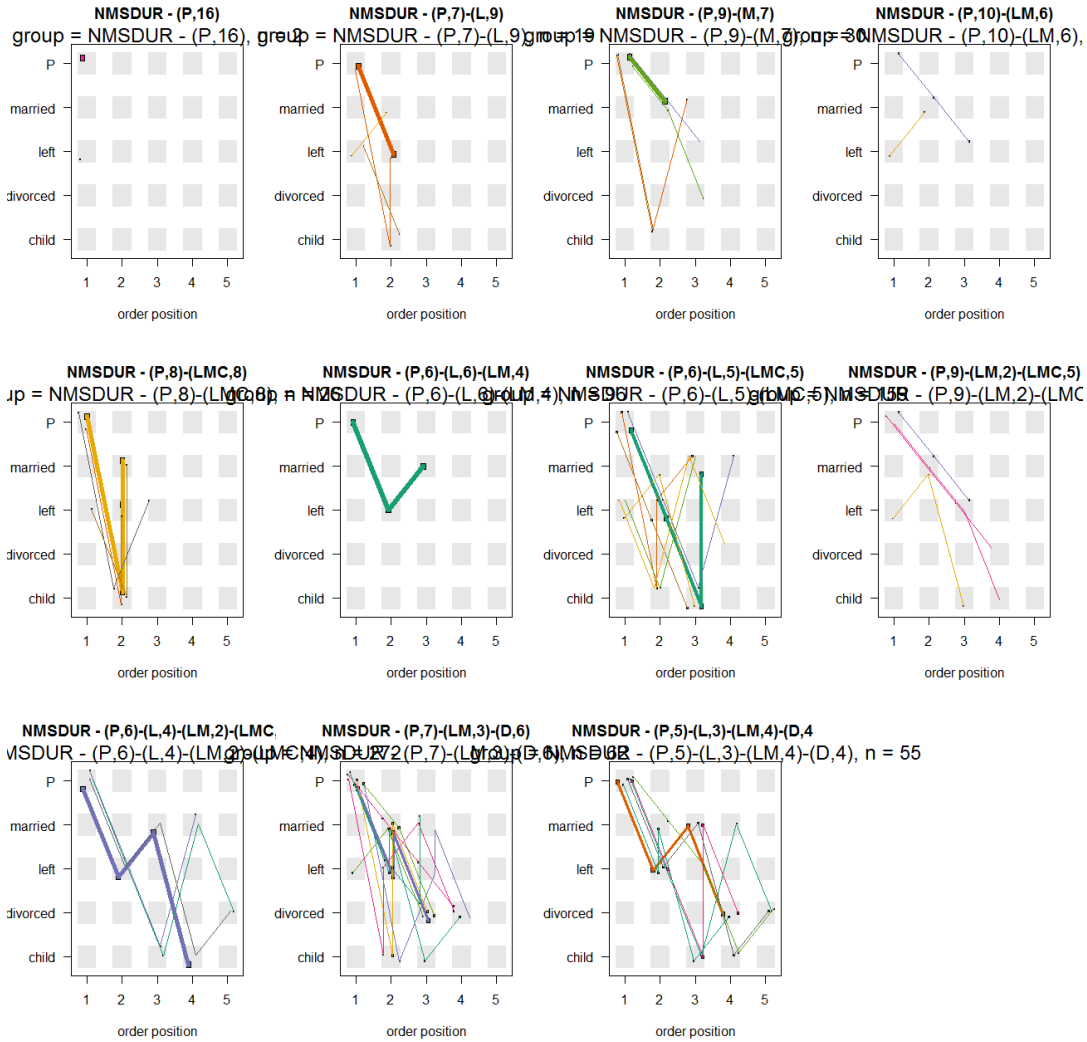


11 clusters seems optimal

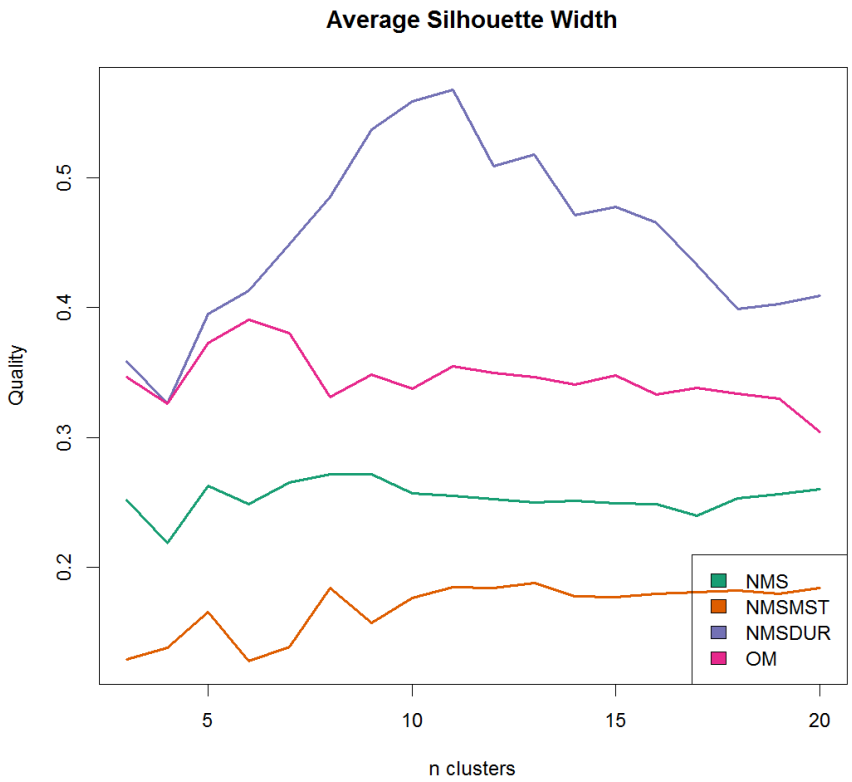
Cluster profiles: Chronogrammes

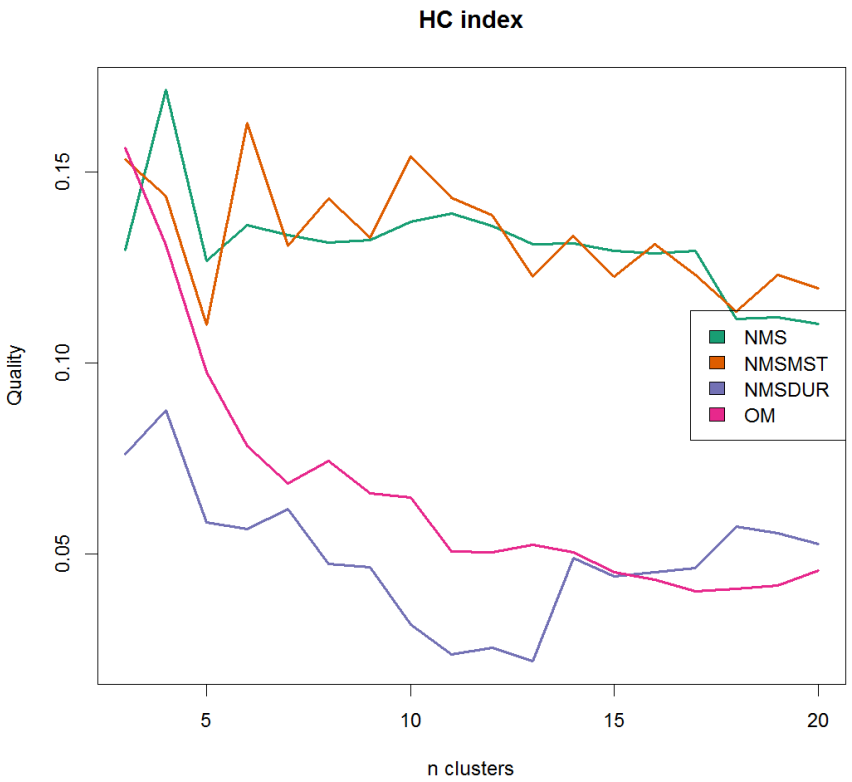


Cluster profiles: order-plots



Clustering Quality





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Choosing Distance is Not Trivial !

Cramer's V: Soft-Matching & OM

	emb	emb/dur	OM
emb	1.0		
emb/dur	.67	1.0	
OM	.84	.65	1.0

THANK YOU

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