WekaBioSimilarity — extending Weka with resemblance measures[*]

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TAMIDA'16

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Introduction

Resemblance-analysis is an important concern in several fields

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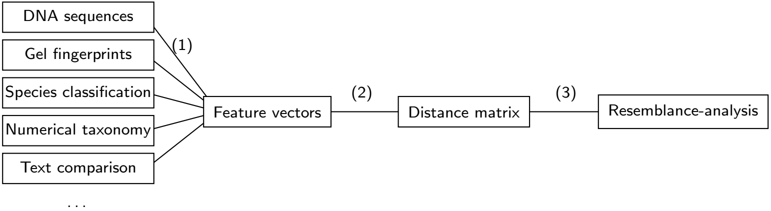

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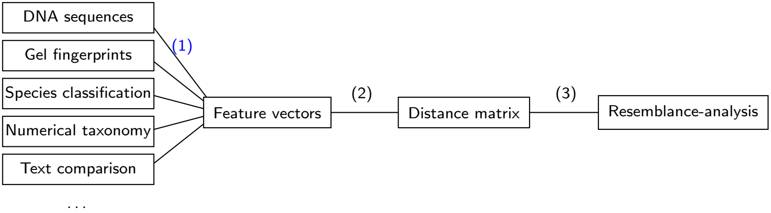
Resemblance-analysis is an important concern in several fields



Depend on the concrete problem

Different types of features: binary, multi-value (nominal), string, or numerical

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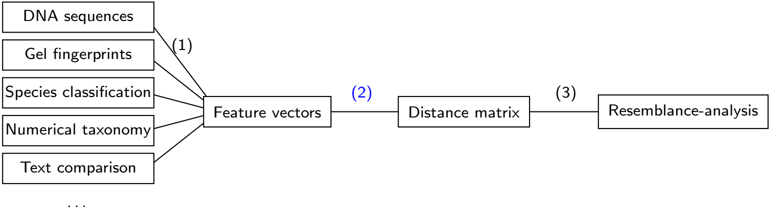

Several resemblance (similarity and distance) measures have been proposed

S. S. Choi et al. *A survey of binary similarity and distance measures*. Journal of Systemics, Cybernetics and Informatics 8(1),43–48. 2010.

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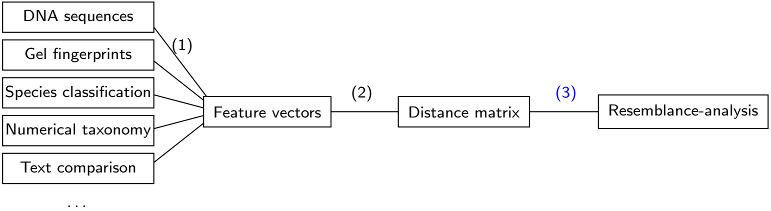

Clustering algorithms

Hierarchical clustering can be visualised using a tree representation

Problem

Several statistical packages (e.g. R, Matlab, Octave, Weka, or SPSS) provide the functionality for resemblance analysis

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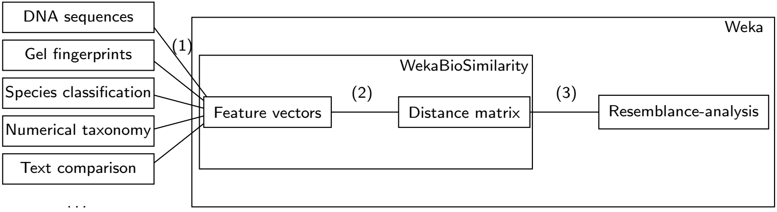
- Problem: they only support binary/or numerical features
- They cannot handle:
  - Comparison of DNA sequences (multi-value/string descriptors)
  - DNA fingerprints (numerical feature vectors)
  - Phylogenetic or data mining (heterogeneous descriptors)
  - . . .

Solution



WekaBioSimilarity:

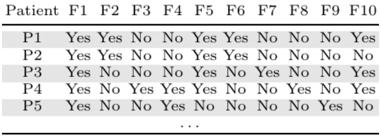
- Extends Weka with resemblance measures and comparison modes
- Works with binary, numerical, nominal, and heterogeneous data
- Open, easily extensible and integrable with other systems

Outline

1. Introduction
2. Resemblance measures in WekaBioSimilarity
3. Integration of WekaBioSimilarity in Weka
4. Conclusions

Binary data

SPECT heart dataset:



Patient	F1	F2	F3	F4	F5	F6	F7	F8	F9	F10
P1	Yes	Yes	No	No	Yes	Yes	No	No	No	Yes
P2	Yes	Yes	No	No	Yes	Yes	No	No	No	No
P3	Yes	No	No	No	Yes	No	Yes	No	No	Yes
P4	Yes	No	Yes	Yes	Yes	No	No	Yes	No	Yes
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					...					

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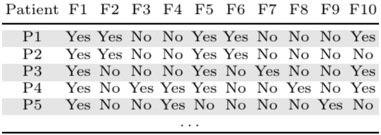

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...										

Given two objects A and B, four values are computed:

- $M_{11} = \sharp$`attributes present both in A and B`
- $M_{10} = \sharp$`attributes present in A but not in B`
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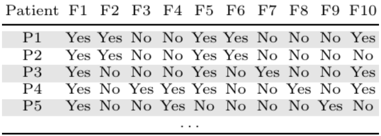

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$$S(A,B) = \frac{M_{11} + M_{00}}{M_{11} + M_{10} + M_{01} + M_{00}}$$

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WekaBioSimilarity features 76 binary resemblance measures

Multi-value/String data — pairwise comparison

HIV-1 protease cleavage dataset:

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- WekaBioSimilarity features 25 resemblance measures (generalised from the binary case)

Multi-value/String data — set occurrence

USDA plants database:

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abelia: fl, nc
abelia x grandiflora: fl, nc
abel.: ct, dc, fl, hi, il, ky, la, md, mi, ms
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- Given A and B, $|S_A \cap S_B|$, $|S_A \setminus S_B|$ and $|S_B \setminus S_A|$ are used to compute resemblance measures:

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- WekaBioSimilarity features 76 resemblance measures (the same as in the binary case)

Numerical data

Three cases:

- Typically: Euclidean distance, Pearson correlation, and so on

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Last two cases only available on WekaBioSimilarity
Notion of closeness: tolerance value

Example: DNA fingerprinting

Comparison of DNA patterns

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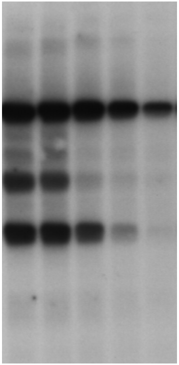

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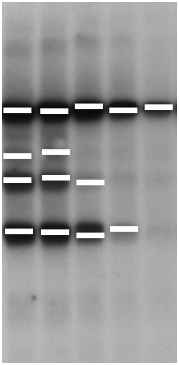

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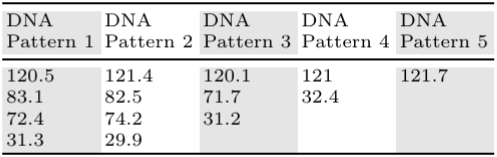

DNA Pattern 1	DNA Pattern 2	DNA Pattern 3	DNA Pattern 4	DNA Pattern 5
120.5	121.4	120.1	121	121.7
83.1	82.5	71.7	32.4	
72.4	74.2	31.2		
31.3	29.9			

Values are different, but they are close enough (tolerance)

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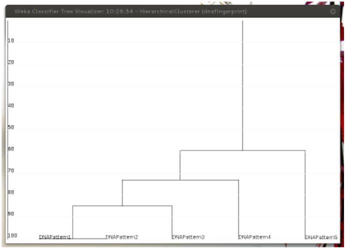
Weka Classifier Tree Visualizer: 10:26:34 - HierarchicalClusterer (dnafingerprint)
10
20
30
40
50
60
70
80
90
100
DNAPattern1
DNAPattern2
DNAPattern3
DNAPattern4
DNAPattern5

Heterogeneous data

Attributes that describe an object may have different types:

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- WekaBioSimilarity implements 25 measures

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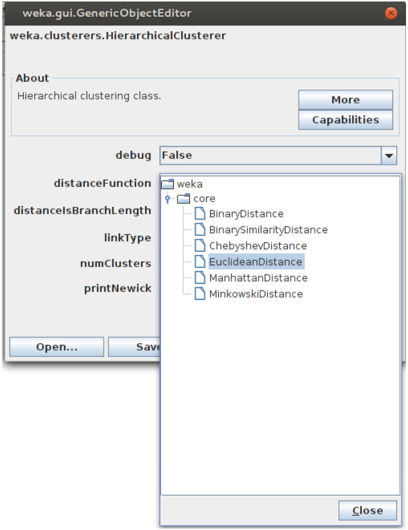
Integration of WekaBioSimilarity in Weka



weka.gui.GenericObjectEditor

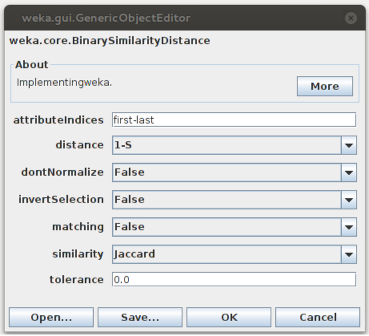
weka.clusterers.HierarchicalClusterer

About

Hierarchical clustering class.

debug: False

Integration of WekaBioSimilarity in Weka



weka.core.BinarySimilarityDistance

About

Implementingweka.

attributeIndices first-last

distance 1-S

dontNormalize False

invertSelection False

matching False

similarity Jaccard

tolerance 0.0

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Resemblance analysis:

- common problem in several contexts
- highly dependent on computing resemblance among objects
- usually special-purpose packages are necessary

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- generalises binary measures to other types of descriptors
- provides tolerance for numerical data
- supports two comparison modes

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WekaBioSimilarity:

- features the same binary measures that other packages
- generalises binary measures to other types of descriptors
- provides tolerance for numerical data
- supports two comparison modes

Result:

- a tool applicable in a wide-variety of problems
- used as a standalone application or integrated in other software

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