An expressive dissimilarity measure for relational clustering using neighbourhood trees

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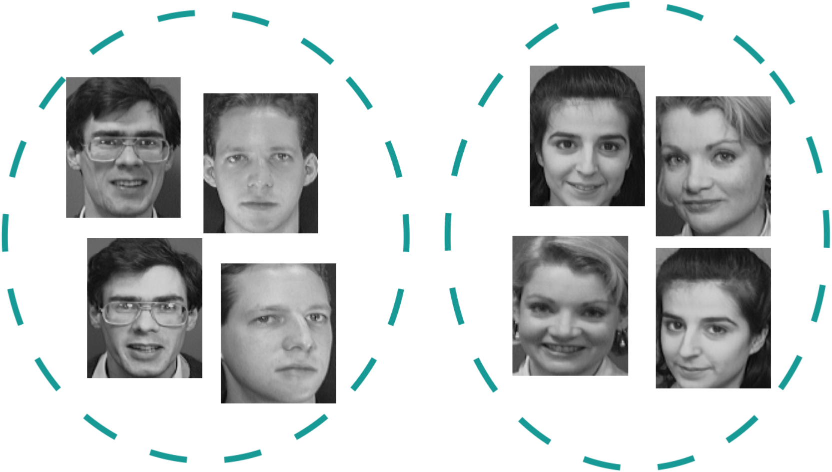
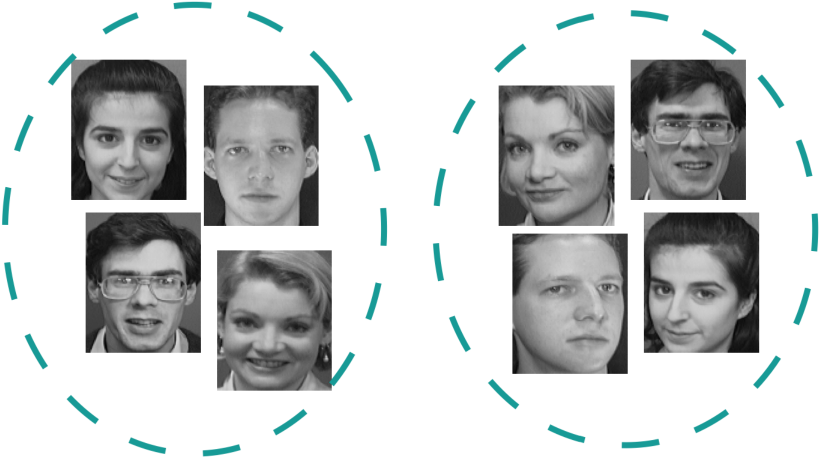
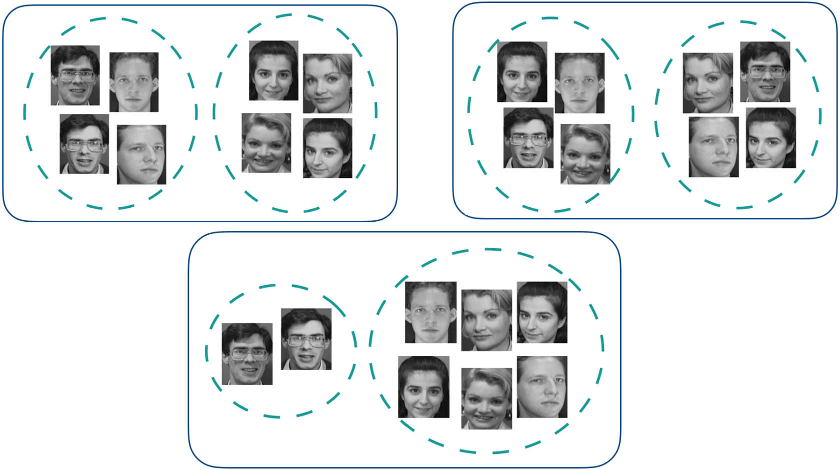
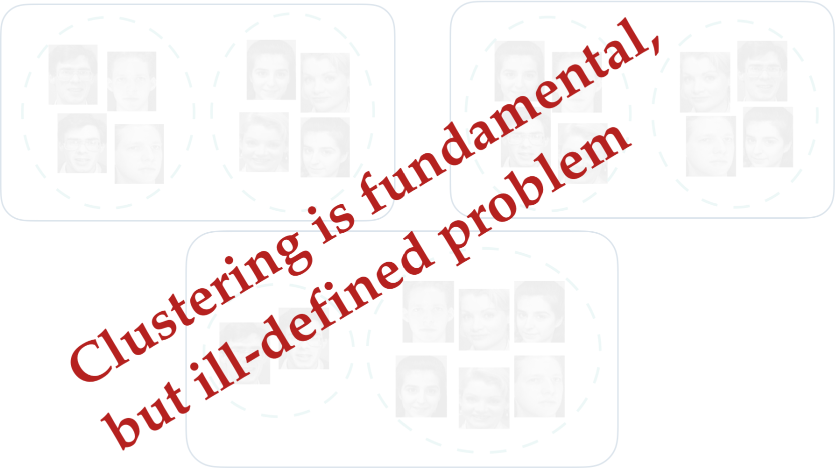




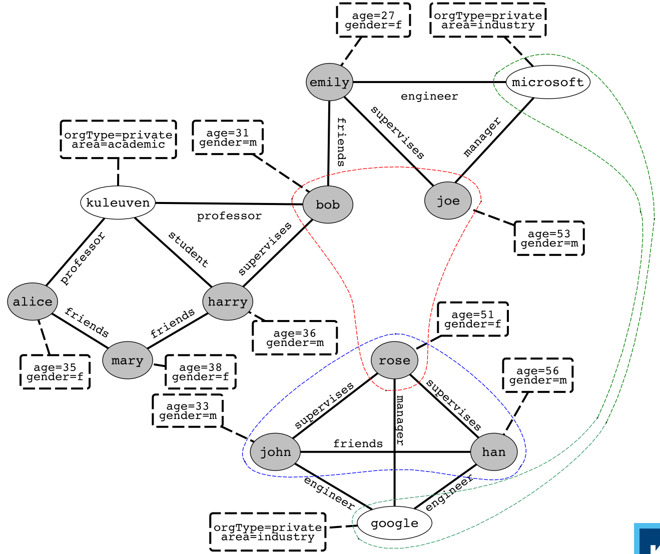
1 – Identifying groups in data





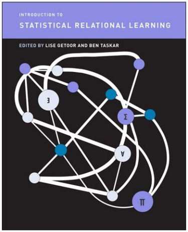
Clustering is fundamental, but ill-defined problem

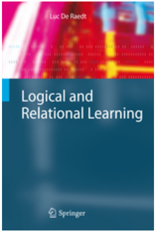
1 – What about relational data?



Machine learning with a powerful knowledge representation language

- usually based on first-order logic





Common representation for:

- vectors
- graphs
- sequences
- ...

... with a unifying reasoning and learning engine a)

```
person(bob,25,m,msc)
person(emily,27,f,msc)
organization(kuleuven,private,academic)
organization(microsoft,private,industry)
friends(bob,emily)
friends(emily,bob)
works_for(bob,kuleuven,professor,2000)
works_for(emily,microsoft,engineer,2300)
```

b)

person

PName	Age	Gender	Education
bob	25	m	msc
emily	27	f	msc

organization

OName	OrgType	Area
kuleuven	private	academic
microsoft	private	industry

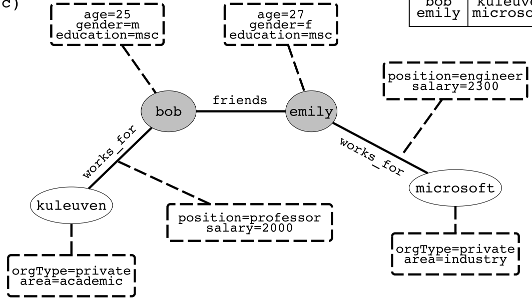
works_for

PName	OName	Position	Salary
bob	kuleuven	professor	2000
emily	microsoft	engineer	2300

friends

PName1	PName2
bob	emily
emily	bob

c)



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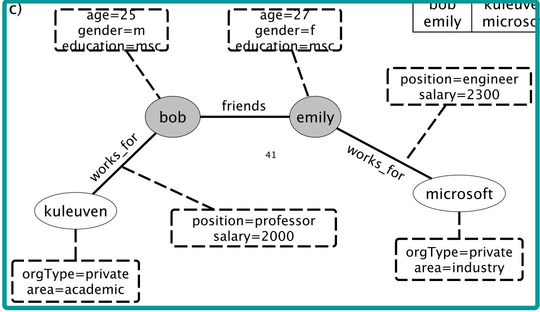

Hybrid similarities	Graph kernels	Relational similarities
incorporate link information into attribute-based similarity	structural similarities of graphs	comparing logical constructs
measure the similarity of connected vertices	*random walks, propagation of information*	*logical formulas in common, matching terms*

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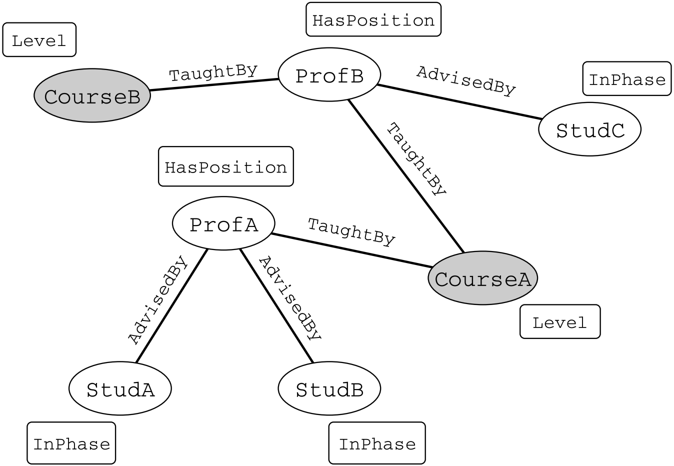
Impose a fixed bias

1. Overture
2. How do we do it now?
3. An expressive dissimilarity for relational data
4. Experiments and results
5. Summary

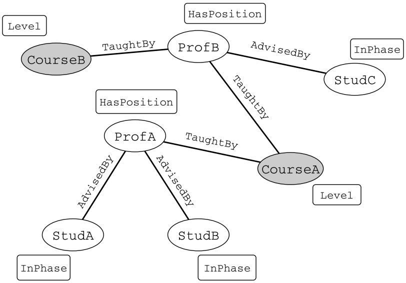
3 – How similar are ProfA and ProfB?



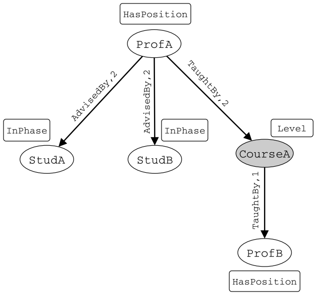
A similarity measure for relational data should:

- incorporate multiple views of similarity
- be easily adaptable
- take attributes and relationships into account
- insensitive to neighbourhood size
- be efficient

Neighbourhood trees summarize the neighbourhood of an instance/example



Data



Neighbourhood tree

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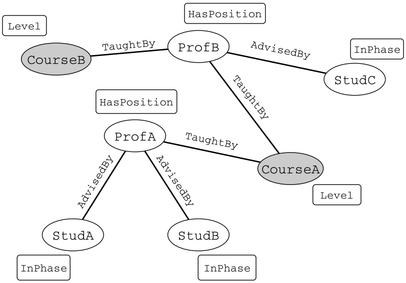
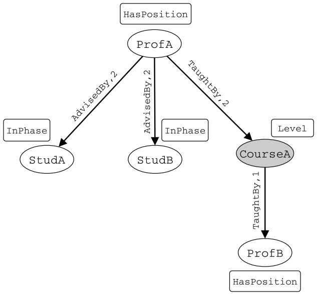


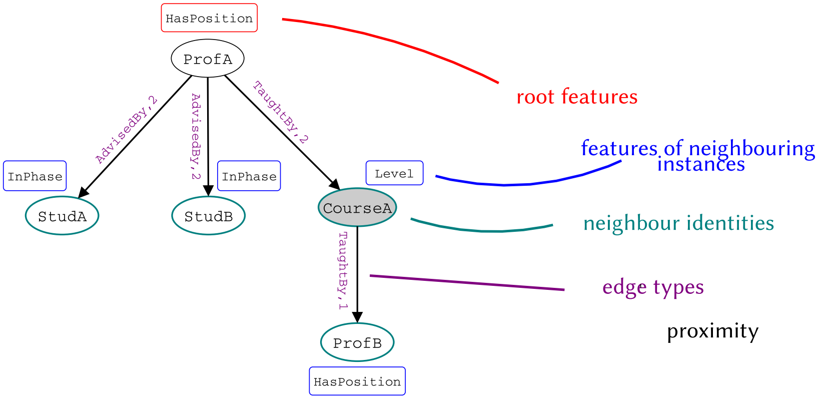
Data



Neighbourhood tree

Similarity of instances = similarity of their neighbourhood trees

Decompose NTs into semantic parts



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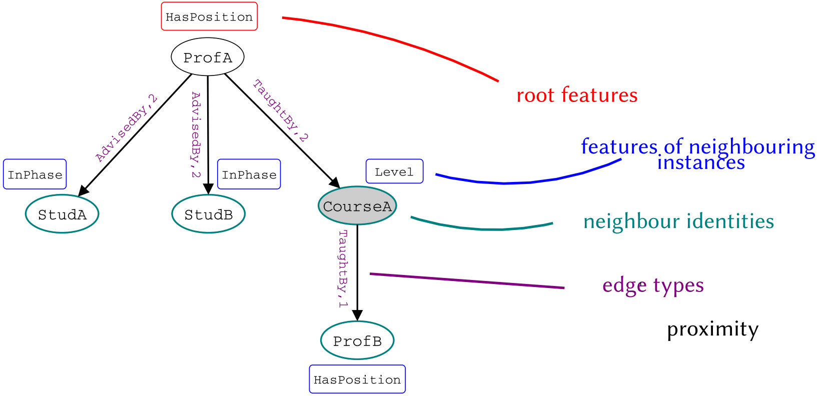
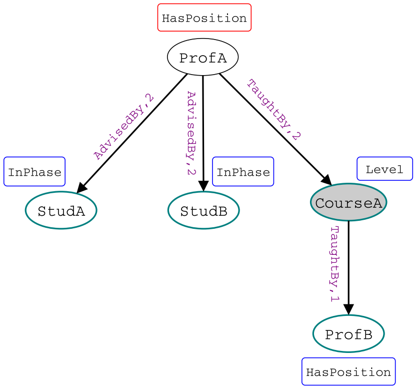


similarity = linear combination of *similarities of individual semantic parts*

$$(w_1, w_2, w_3, s_4, w_5)$$



Decompose NT in multisets of:

- attribute
- edge labels
- vertex identities

per level and vertex type

Multiset of edge labels (level 1):
{ (Advised,2), (Advised,2), (TaughtBy,2) }

Compare two multisets, A and B with χ^2 distance

$$\chi^2(A,B) = \sum_{x \in A \cup B} \frac{(f_A(x) - f_B(x))^2}{f_A(x) + f_B(x)}$$

Many of the existing similarities are a special case:

- hybrid similarities
- relational similarities

... or they can be defined over neighbourhood trees (graph kernels) with different biases:

- makes it easier to compare the imposed biases

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Additionally: effective - linear in the number of unique elements in a multiset

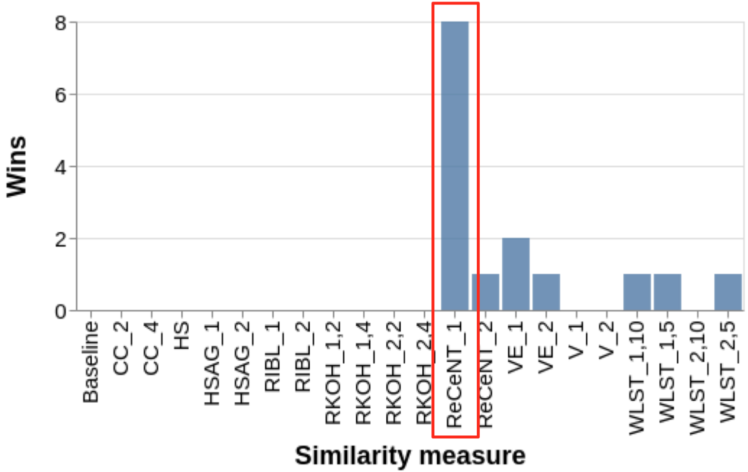
Datasets:

- IMDB
- UWCSE
- Mutagenesis
- WebKB
- TerroristAttacks

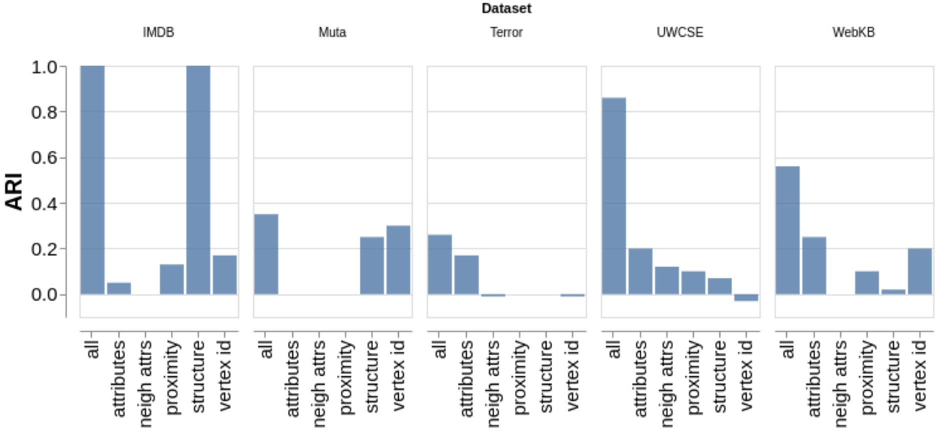
Questions:

- *Quality of the obtained clustering?*
- *Are different views really necessary?*
- *Can we learn the bias from data?*
- *Can we learn the bias from labels?*

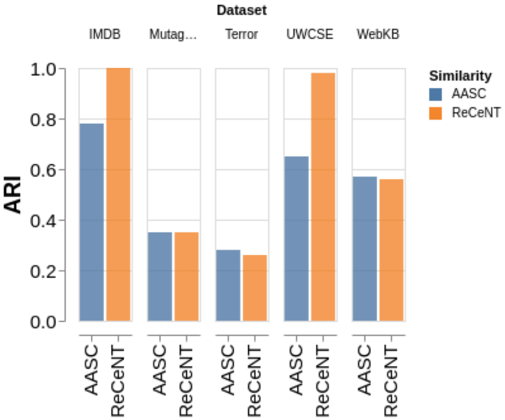
- combined with spectral and hierarchical clustering
- a wide range of existing similarity measures
- performance measure: ARI/Accuracy



Takeaway message: incorporating multiple biases consistently performs well



Takeaway message: relational data requires multiple views of similarity in order to find informative clusters



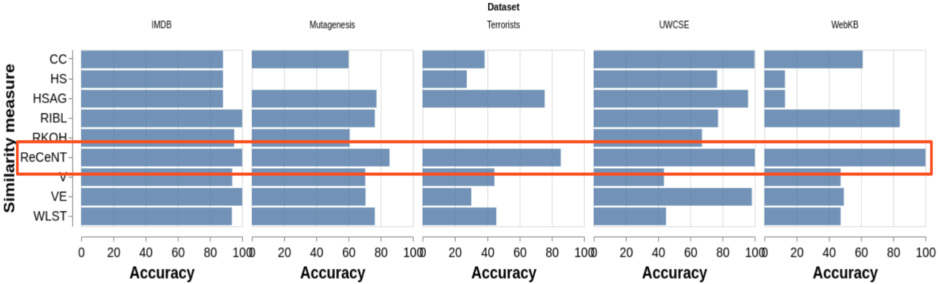
`ReCeNT` with $w_i = 0.2$
vs.
AASC + `ReCeNT`

AASC - given multiple similarity matrices, find an optimal combination for clustering

barely any benefit

Huang, Chuang, Chen: Affinity Aggregation for Spectral Clustering

Similarity measure in combination with a kNN (parameters optimised with CV)



Takeaway message: when labels are provided, `ReCeNT` outperforms the competing similarities

A similarity measure for relational data that:

- is versatile (meta-similarity)
- easily adaptable
- efficient
- generalization of many existing structured/relational sims
- works well across many different tasks

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Code: `https://dtai.cs.kuleuven.be/software/recent`

S. Dumancic, H. Blockeel: *Clustering-Based Unsupervised Relational Representation Learning with an Explicit Distributed Representation*, IJCAI '17

S. Dumancic, H. Blockeel: *Demystifying Relational Latent Representations*, ILP '17