

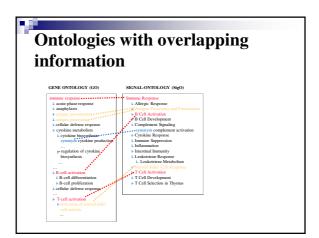
Ontology Alignment

- n Ontology alignment
- n Ontology alignment strategies
- n Evaluation of ontology alignment strategies
- Recommending ontology alignment strategies
- n Using PRA in ontology alignment
- n Current issues

Ontologies in biomedical research

- n many biomedical ontologies e.g. GO, OBO, SNOMED-CT
- practical use of biomedical ontologies
 - e.g. databases annotated with GO

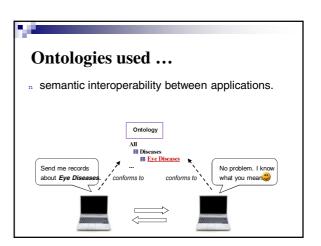


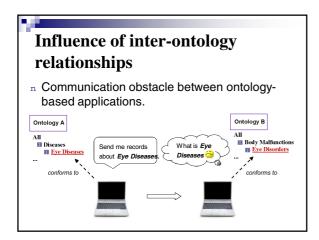


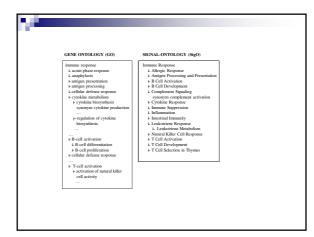
Ontologies with overlapping information

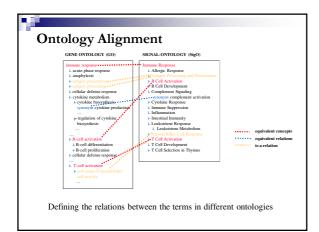
- n Use of multiple ontologies
 - □ custom-specific ontology + standard ontology
 - ¤ different views over same domain
 - overlapping domains
- Bottom-up creation of ontologies experts can focus on their domain of expertise

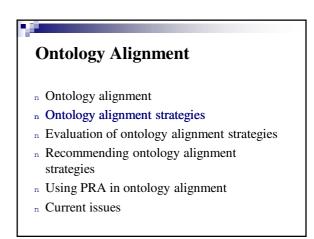
important to know the inter-ontology relationships

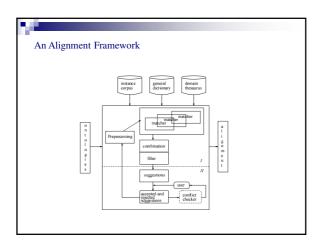




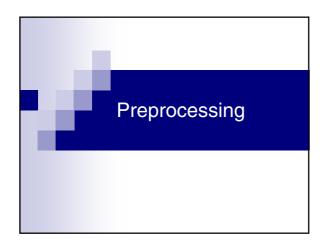


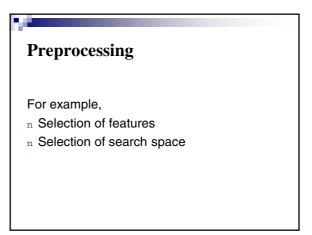


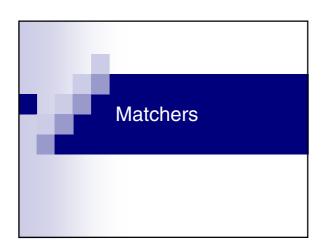


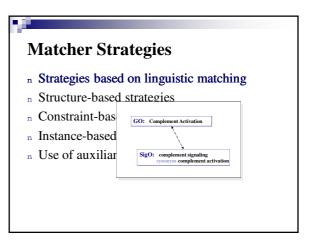


Classification n According to input KR: OWL, UML, EER, XML, RDF, ... components: concepts, relations, instance, axioms According to process What information is used and how? According to output 1-1, m-n Similarity vs explicit relations (equivalence, is-a) confidence









Example matchers

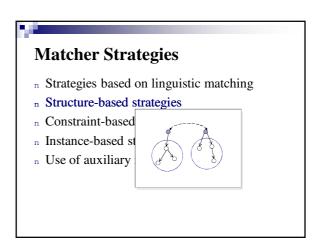
n Edit distance

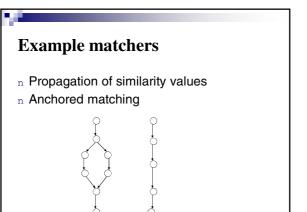
Number of deletions, insertions, substitutions required to transform one string into another

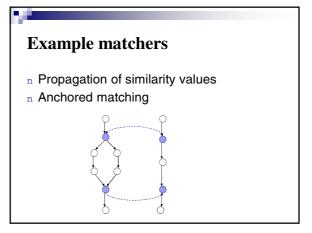
aaaa baab: edit distance 2

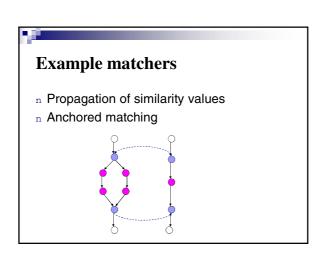
n N-gram

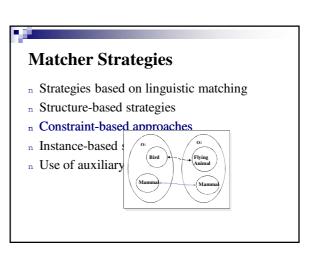
N-gram: N consecutive characters in a string
Similarity based on set comparison of n-grams
aaaa: {aa, aa, aa}; baab: {ba, aa, ab}











Matcher Strategies n Strategies based on linguistic matching n Structure-based strategies n Constraint-based approaches n Instance-based n Use of auxiliary

Matcher Strategies

- n Strategies based on linguisti
- n Structure-based strategies
- n Constraint-based approaches
- n Instance-based strategies
- n Use of auxiliary information





Example matchers

- n Instance-based
- n Use life science literature as instances
- n Structure-based extensions

Learning matchers – instancebased strategies

- n Basic intuition
 - A similarity measure between concepts can be computed based on the probability that documents about one concept are also about the other concept and vice versa.
- n Intuition for structure-based extensions Documents about a concept are also about their super-concepts.

(No requirement for previous alignment results.)

Learning matchers - steps

- n Generate corpora
 - Use concept as query term in PubMed
 - Retrieve most recent PubMed abstracts
- n Generate text classifiers
 - u One classifier per ontology / One classifier per concept
- Classification
 - Abstracts related to one ontology are classified by the other ontology's classifier(s) and vice versa
- n Calculate similarities



Basic Naïve Bayes matcher

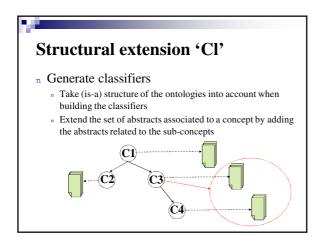
- n Generate corpora
- n Generate classifiers
 - Naive Bayes classifiers, one per ontology
- n Classification
 - Abstracts related to one ontology are classified to the concept in the other ontology with highest posterior probability P(Cld)
- n Calculate similarities

$$sim(C_1, C_2) = \frac{n_{NBC2}(C_1, C_2) + n_{NBC1}(C_2, C_1)}{n_D(C_1) + n_D(C_2)}$$

Basic Support Vector Machines matcher

- n Generate corpora
- n Generate classifiers
 - SVM-based classifiers, one per concept
- n Classification
 - Single classification variant: Abstracts related to concepts in one ontology are classified to the concept in the other ontology for which its classifier gives the abstract the highest positive value.
 - Multiple classification variant: Abstracts related to concepts in one ontology are classified all the concepts in the other ontology whose classifiers give the abstract a positive value.
- n Calculate similarities

$$\frac{n_{SVMC-C_2}(C_1,C_2) + n_{SVMC-C_1}(C_2,C_1)}{n_D(C_1) + n_D(C_2)}$$



Structural extension 'Sim'

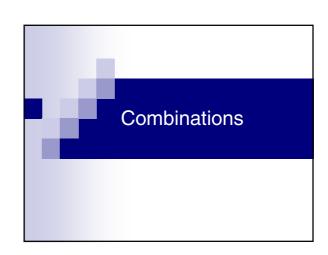
- n Calculate similarities
 - Take structure of the ontologies into account when calculating similarities
 - Similarity is computed based on the classifiers applied to the concepts and their sub-concepts

$$sim_{struct}(C_1,C_2) = \frac{\sum_{C_i \subseteq C_1, C_j \subseteq C_2} n_{NBC2}(C_i,C_j) + \sum_{C_i \subseteq C_1, C_j \subseteq C_2} n_{NBC1}(C_j,C_i)}{\sum_{C_i \subseteq C_1} n_D(C_i) + \sum_{C_j \subseteq C_2} n_D(C_j)}$$

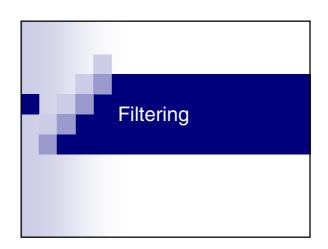
Matcher Strategies n Strategies based linguist n Structure-based strategie n Constraint-based approa n Instance-based strategies n Use of auxiliary information

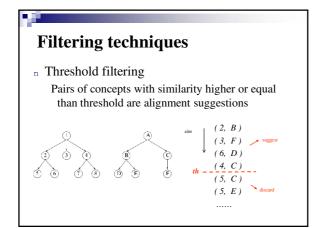
Example matchers n Use of WordNet use WordNet to find synonyms use WordNet to find ancestors and descendants in the isa hierarchy use of Unified Medical Language System (UMLS) Includes many ontologies Includes many alignments (not complete) use UMLS alignments in the computation of the similarity values

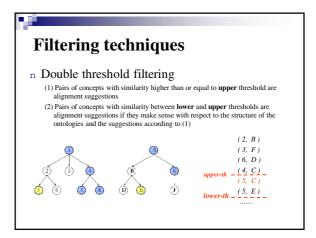
	linguistic	structure	constraints	instances	auxiliary
ArtGen	name	parents, children	Constituints	domain	WordNet
	- manie	parents, emiaren		specific	Wordstee
				documents	
ASCO	name,	parents, children,			WordNet
	label	siblings,			
	description	path from root			
Chimaera	name	parents, children			
FCA-Merge	name			domain	
				specific	
				documents	
FOAM	name,	parents, children	equivalence		
	label				
GLUE	name	neighborhood		instances	
HCONE	name	parents, children			WordNet
	l manne	parento, emiaren			
IF-Map				instances	a reference
					ontology
iMapper		leaf, non-leaf,	domain,	instances	WordNet
		children,	range		
		related node			
OntoMapper		parents, children		documents	
(Anchor-)	name	direct graphs			
PROMPT					
SAMBO	name,	is-a and part-of,		domain	WordNet,
	synonym	descendants		specific	UMLS
		and ancestors		documents	
S-Match	label	path from root	semantic		WordNet
	l	1	relations		1
	l	1	codified		1
	I	1	in labels		I

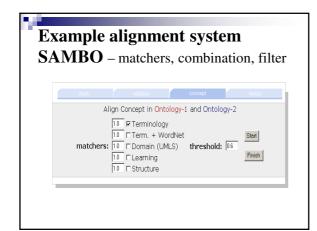


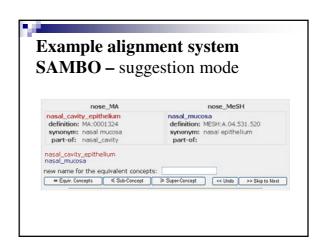
Combination Strategies n Usually weighted sum of similarity values of different matchers n Maximum of similarity values of different matchers

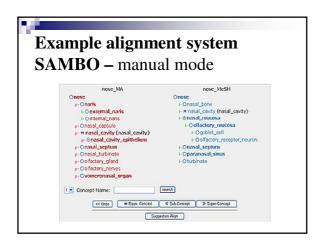






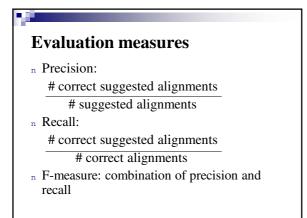






Ontology Alignment

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OAEI

- n Since 2004
- n Evaluation of systems
- n Different tracks
 - comparison: benchmark (open)
 - expressive: anatomy (blind), fisheries (expert)
 - directories and thesauri: directory, library, crosslingual resources (blind)
 - consensus: conference

OAEI

- n Evaluation measures
 - Precision/recall/f-measure
 - * recall of non-trivial mappings
 - full / partial golden standard

OAEI 2007

- _n 17 systems participated
 - benchmark (13)
 - n ASMOV: p = 0.95, r = 0.90
 - anatomy (11)
 - n AOAS: f = 0.86, r+ = 0.50
 - n SAMBO: f =0.81, r+ = 0.58
 - library (3)
 - n Thesaurus merging: FALCON: p = 0.97, r = 0.87
 - n Annotation scenario:
 - FALCON: pb =0.65, rb = 0.49, pa = 0.52, ra = 0.36, Ja = 0.30
 - Silas: pb = 0.66, rb= 0.47, pa = 0.53, ra = 0.35, Ja = 0.29
 - directory (9), food (6), environment (2), conference (6)

OAEI 2008 – anatomy track

- n Align
 - Mouse anatomy: 2744 terms
 - NCI-anatomy: 3304 terms
 - Mappings: 1544 (of which 934 'trivial')
- n Tasks
 - 1. Align and optimize f
 - ≈ 2-3. Align and optimize p / r
 - 4. Align when partial reference alignment is given and optimize f

OAEI 2008 - anatomy track#1

- _n 9 systems participated
- n SAMBO
 - = p=0.869, r=0.836, r+=0.586, f=0.852
- n SAMBOdtf
 - p=0.831, r=0.833, r+=0.579, f=0.832
- n Use of TermWN and UMLS

OAEI 2008 – anatomy track#1

Is background knowledge (BK) needed?

Of the non-trivial mappings:

- $^{\scriptscriptstyle \rm I\hspace{-1pt}I}$ Ca 50% found by systems using BK and systems not using BK
- Ca 13% found only by systems using BK
- E Ca 13% found only by systems not using BK
- Ca 25% not found

Processing time:

hours with BK, minutes without BK

OAEI 2008 - anatomy track#4

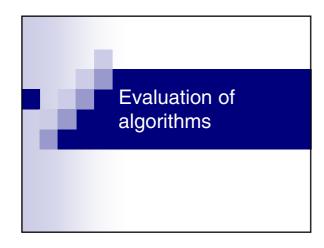
Can we use given mappings when computing suggestions? partial reference alignment given with all trivial and 50 non-trivial mappings

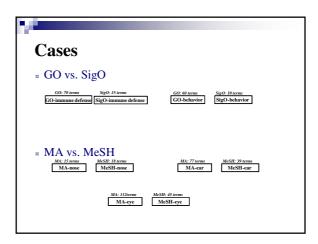
- n SAMBO
 - p=0.636 0.660, r=0.626 0.624, f=0.631 0.642
- n SAMBOdtf
 - p=0.563 0.603, r=0.622 0.630, f=0.591 0.616

(measures computed on non-given part of the reference alignment)

OAEI 2007-2008

- Systems can use only one combination of strategies per task
 - systems use similar strategies
 - text: string matching, tf-idf
 - structure: propagation of similarity to ancestors and/or descendants
 - * thesaurus (WordNet)
 - domain knowledge important for anatomy task?



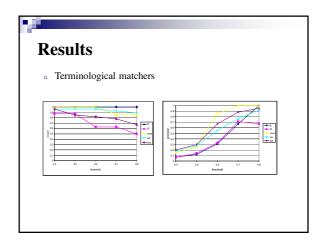


Evaluation of matchers

Matchers
Term, TermWN, Dom, Learn (Learn+structure), Struc

Parameters
Quality of suggestions: precision/recall
Threshold filtering: 0.4, 0.5, 0.6, 0.7, 0.8
Weights for combination: 1.0/1.2

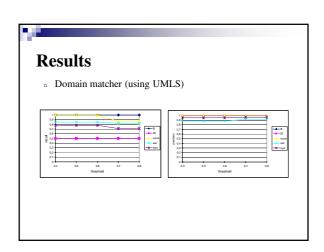
KitAMO
(http://www.ida.liu.se/labs/iislab/projects/KitAMO)



Results

n Basic learning matcher (Naïve Bayes)

Naive Bayes slightly better recall, but slightly worse precision than SVM-single SVM-multiple (much) better recall, but worse precision than SVM-single



Results

n Comparison of the matchers

 $CS_TermWN \supseteq CS_Dom \supseteq CS_Learn$

- Combinations of the different matchers
 - n combinations give often better results
 - n no significant difference on the quality of suggestions for different weight assignments in the combinations

(but: did not check yet for large variations for the weights)

Structural matcher did not find (many) new correct alignments
 (but: good results for systems biology schemas SBML – PSI MI)

Evaluation of filtering

n Matcher

TermWN

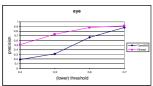
n Parameters

Quality of suggestions: precision/recall Double threshold filtering using structure:

Upper threshold: 0.8

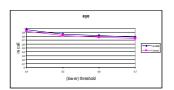
Lower threshold: 0.4, 0.5, 0.6, 0.7, 0.8

Results



The precision for double threshold filtering with upper threshold 0.8 and lower threshold T is higher than for threshold filtering with threshold T

Results



The recall for double threshold filtering with upper threshold 0.8 and lower threshold T is about the same as for threshold filtering with threshold T

Ontology Alignment

- n Ontology alignment
- n Ontology alignment strategies
- n Evaluation of ontology alignment strategies
- Recommending ontology alignment strategies
- $_{\mbox{\tiny n}}$ Using PRA in ontology alignment
- n Current issues

Recommending strategies - 1

- n Use knowledge about previous use of alignment strategies
 - gather knowledge about input, output, use, performance, cost via questionnaires
 - x Not so much knowledge available
 - **¤** OAEI

(Mochol, Jentzsch, Euzenat 2006)

Recommending strategies - 2

- n Optimize
 - Parameters for ontologies, similarity assessment, matchers, combinations and filters
 - Run general alignment algorithm
 - user validates the alignment result
 - Optimize parameters based on validation

(Ehrig, Staab, Sure 2005)

Recommending strategies - 2

- n Tests
 - travel in russia
 QOM: r=0.618, p=0.596, f=0.607
 Decision tree 150: r=0.723, p=0.591, f=0.650
 - bibster
 QOM: r=0.279, p=0.397, f=0.328
 Decision tree 150: r=0.630, p=0.375, f=0.470

Decision trees better than Neural Nets and Support Vector Machines.

Recommending strategies - 3

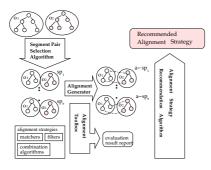
- n Based on inherent knowledge
 - use the actual ontologies to align to find good candidate alignment strategies
 - user/oracle with minimal alignment work
 - Complementary to the other approaches

(Tan, Lambrix 2007)

Idea

- n Select small segments of the ontologies
- n Generate alignments for the segments (expert/oracle)
- n Use and evaluate available alignment algorithms on the segments
- n Recommend alignment algorithm based on evaluation on the segments

Framework



Experiment case





- n NCI thesaurus
 - National Cancer Institute, Center for Bioinformatics
 - Anatomy: 3495 terms
- n MeSH
 - x National Library of Medicine
 - Anatomy: 1391 terms

Experiment case - Oracle

- n UMLS
 - Library of Medicine

 - NCI thesaurus and MeSH included in UMLS
 - Used as approximation for expert knowledge
 - □ 919 expected mappings according to UMLS

Experiment case

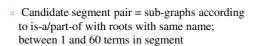
- alignment strategies

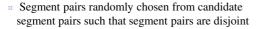
- n Matchers and combinations
 - N-gram (NG)
 - Edit Distance (ED)
 - Word List + stemming (WL)
 - Word List + stemming + WordNet (WN)
 - NG+ED+WL, weights 1/3 (C1)

 ■
 - x NG+ED+WN, weights 1/3 (C2)
- n Threshold filter
 - thresholds 0.4, 0.5, 0.6, 0.7, 0.8

Segment pair selection algorithms



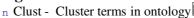


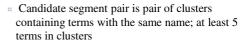






Segment pair selection algorithms





Segment pairs randomly chosen from candidate segment pairs





Segment pair selection algorithms

- $_{\rm n}\,$ For each trial, 3 segment pair sets with 5 segment pairs were generated
- n SubG: A1, A2, A3
 - 2 to 34 terms in segment
 - □ level of is-a/part-of ranges from 2 to 6
 - max expected alignments in segment pair is 23
- n Clust: B1, B2, B3
 - 5 to 14 terms in segment
 - □ level of is-a/part-of is 2 or 3
 - max expected alignments in segment pair is 4

Segment pair alignment generator

n Used UMLS as oracle

Agency design of the control of the

Alignment toolbox

n Used KitAMO as toolbox



Generates reports on similarity values produced by different matchers, execution times, number of correct, wrong, redundant suggestions

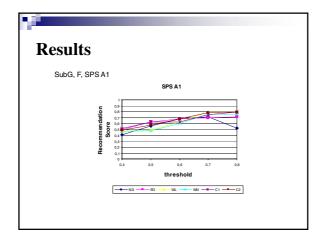
Recommendation algorithm



- n Recommendation scores: F, F+E, 10F+E
- F: quality of the alignment suggestions
 - average f-measure value for the segment pairs
- E: average execution time over segment pairs, normalized with respect to number of term pairs
- Algorithm gives ranking of alignment strategies based on recommendation scores on segment pairs

Expected recommendations for F

- Best strategies for the whole ontologies and measure F:
- 1. (WL,0.8)
- 2. (C1,0.8)
- 3. (C2,0.8)



Results

- Top 3 strategies for SubG and measure F:
- A1: 1. (WL,0.8) (WL, 0.7) (C1,0.8) (C2,0.8)
- A2: 1. (WL,0.8) 2. (WL,0.7) 3. (WN,0.7)
- A3: 1. (WL,0.8) (WL, 0.7) (C1,0.8) (C2,0.8)
- Best strategy always recommended first
- n Top 3 strategies often recommended
- n (WL,0.7) has rank 4 for whole ontologies

Results

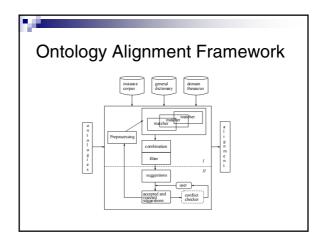
- Top 3 strategies for Clust and measure F:
- B1: 1. (C2,0.7) 2. (ED,0.6) 3. (C2,0.6)
- B2: 1. (WL,0.8) (WL, 0.7) (C1,0.8) (C2,0.8)
- B3: 1. (C1,0.8) (ED,0.7) 3. (C1,0.7) (C2,0.7) (WL,0.7) (WN,0.7)
- n Top strategies often recommended, but not always
- n (WL,0.7) (C1,0.7) (C2,0.7) ranked 4,5,6 for whole ontologies

Results

- SubG gives better results than Clust
- n Results improve when number of segments is increased
- n 10F+E similar results as F
- _n F+F
 - wordNet gives lower ranking
 - Runtime environment has influence

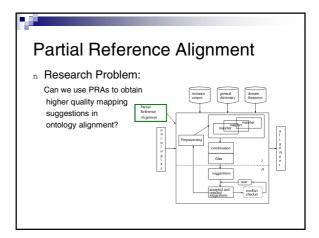
Ontology Alignment

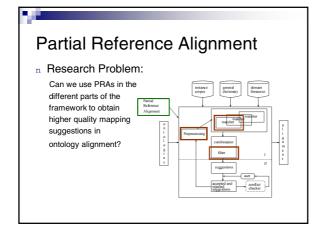
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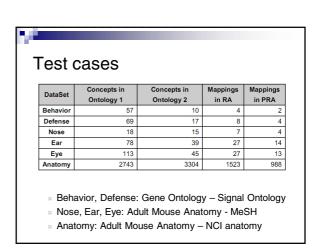


Partial Reference Alignment

- n New setting for ontology alignment:
 - Portals with mappings
 - Iterative ontology alignment
 - Anatomy track, task 4 in OAEI 2008
 In all these cases some correct mappings between terms in different ontologies are given or have been obtained.
- $_{\rm n}~$ A partial reference alignment (PRA) is a subset of all correct mappings.

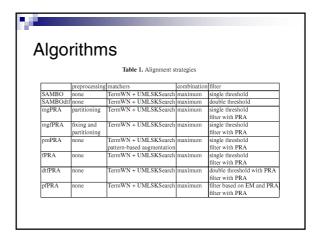


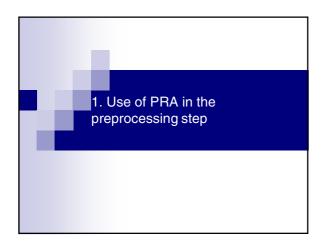


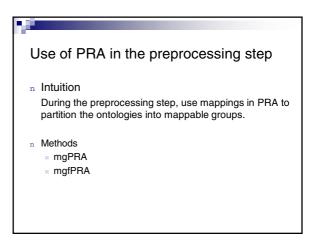


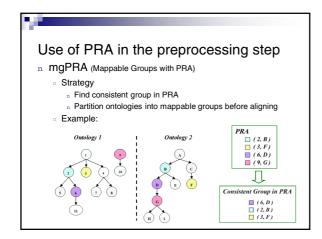
Evaluation

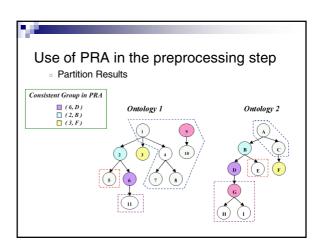
- $_{\rm n}$ Precision: number of correct suggestions divided by number of suggestions
- $_{\rm n}$ $\it Recall: {\rm number}$ of correct suggestions divided by number of correct mappings
- n Recall-PRA: number of correct suggestions not in PRA divided by number of correct mappings not in PRA
- n F-measure: harmonic mean of precision and recall

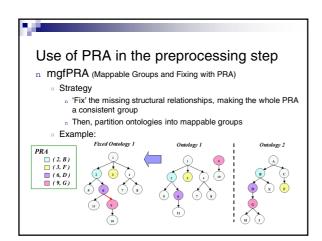


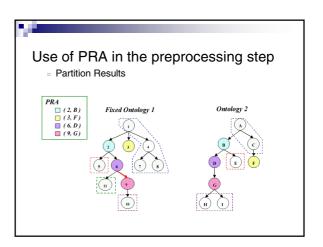






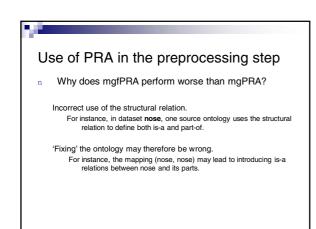


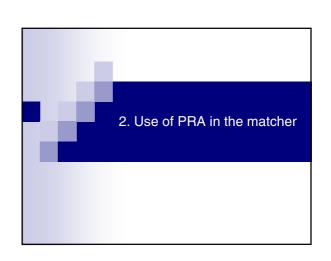


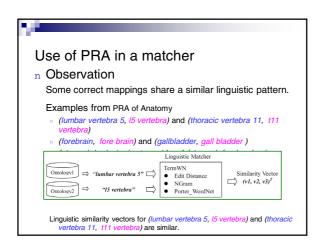


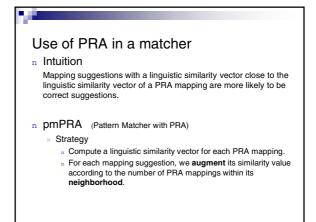
Use of PRA in the preprocessing step

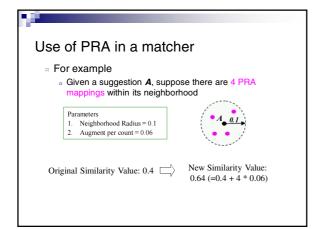
Result Analysis
For threshold 0.4, there are no conclusive results.
For thresholds 0.6 and 0.8,
mgPRA and mgfPRA almost always have equal or higher precision than SAMBO.
mgPRA almost always has equal or higher recall than SAMBO.
mgfPRA almost always has equal or lower recall than SAMBO and mgPRA.

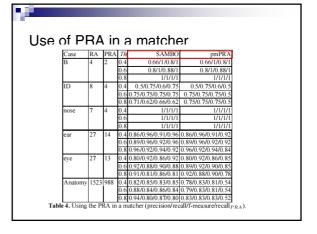


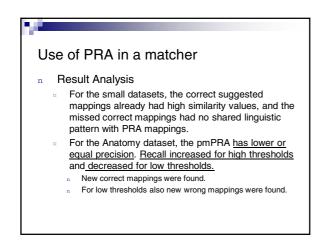


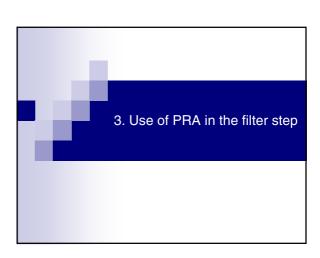


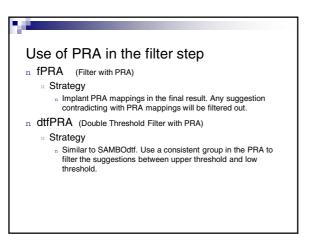


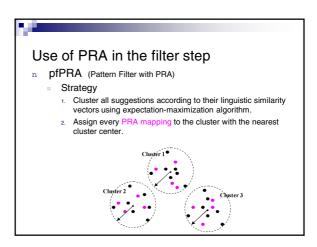


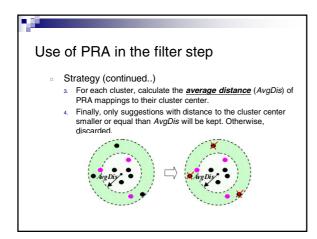


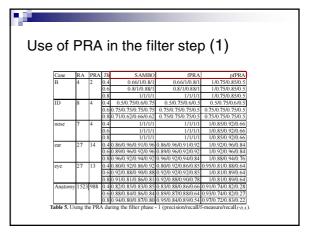






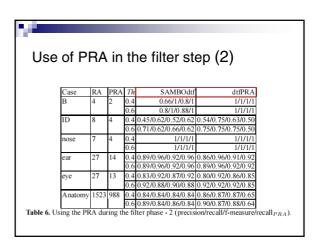






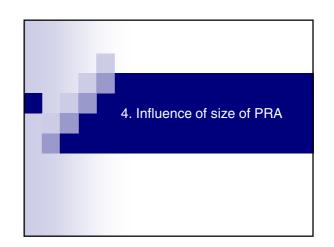
Use of PRA in the filter step (1)

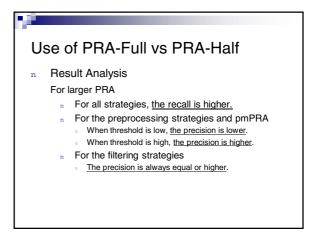
- n Result Analysis
 - ¹² fPRA always has <u>equal or higher precision</u> <u>and recall</u> than SAMBO.
 - pfPRA always has <u>equal or higher precision</u> than fPRA and SAMBO.
 - pfPRA always has <u>equal or lower recall</u> than SAMBO.
 - Some correct suggestions are filtered out because they have no similar linguistic pattern to PRA mappings.

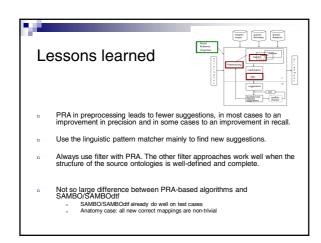


Use of PRA in the filter step (2)

- n Result Analysis
 - dtfPRA always has <u>equal or higher recall</u> than SAMBOdtf.
 - For lower threshold 0.6, dtfPRA always has equal or higher precision than SAMBOdtf.
 - For lower threshold 0.4, dtfPRA always has <u>equal or higher precision</u> than SAMBOdtf, except for dataset <u>ear</u> and <u>eve</u>.
 - n For dataset **ear** and **eye**, the consistent group of dtfPRA is much smaller than the consistent group of SAMBOdtf.







Ontology Alignment n Ontology alignment n Ontology alignment strategies n Evaluation of ontology alignment strategies n Recommending ontology alignment strategies n Using PRA in ontology alignment n Current Issues

Current issues

- n Systems and algorithms
 - Complex ontologies
 - use of instance-based techniques
 - Alignment types (equivalence, is-a, ...)
 - □ Complex mappings (1-n, m-n)
 - □ Connection ontology types alignment strategies

Current issues

- n Evaluations
 - Need for Golden standards
 - Systems available, but not always the alignment algorithms
 - Evaluation measures
- n Recommending 'best' alignment strategies

Further reading

Starting points for further studies



Further reading ontology alignment

- n <u>http://www.ontologymatching.org</u> (plenty of references to articles and systems)
- $\tt n$. Ontology alignment evaluation initiative: $\underline{\tt http://oaei.ontologymatching.org}$ (home page of the initiative)
- n Euzenat, Shvaiko, Ontology Matching, Springer, 2007.
- n Lambrix, Tan, SAMBO a system for aligning and merging biomedical ontologies, Journal of Web Semantics, 4(3):196-206, 2006.
- (description of the SAMBO tool and overview of evaluations of different matchers)
- Lambrix, Tan, A tool for evaluating ontology alignment strategies, Journal on Data Semantics, VIII:182-202, 2007.
 (description of the KitAMO tool for evaluating matchers)

Further reading ontology alignment

Chen, Tan, Lambrix, Structure-based filtering for ontology alignment, IEEE WETICE workshop on semantic technologies in collaborative applications, 364-

(double threshold filtering technique)

- Tan, Lambrix, A method for recommending ontology alignment strategies, International Semantic Web Conference, 494-507, 2007.
 Ehrig, Staab, Sure, Bootstrapping ontology alignment methods with APFEL, International Semantic Web Conference, 186-200, 2005.
 Mochol, Jentzsch, Euzenat, Applying an analytic method for matching approach selection, International Workshop on Ontology Matching, 2006.
 (recommendation of alignment strategies)
- Lambrix, Liu, Using partial reference alignments to align ontologies, European Semantic Web Conference, 188-202, 2009.
 (PRA in ontology alignment)

Further reading ontology alignment

Lambrix, Strömbäck, Tan, Information integration in bioinformatics with ontologies and standards, chapter 8 in Bry, Maluszynski (eds), Semantic Techniques for the Web, Springer, 2009. ISBN: 978-3-642-04580-6. (largest overview of systems)

