DATA LINKING AND KNOWLEDGE DISCOVERY IN RDF DATA: METHODS AND SOME FEEDBACK FROM AGRONOMIC APPLICATIONS

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LAHDAK@LRI, PARIS SUD UNIVERSITY, CNRS, PARIS SACLAY UNIVERSITY Joint work with: N. Pernelle, L. Papaleo, J. Raad and D. Symeonidou

1st DATAIA DAYS « LIFE SCIENCES & AI», DEC. 4TH 2019







Comprendre le monde, construire l'avenir®



LINKED OPEN DATA

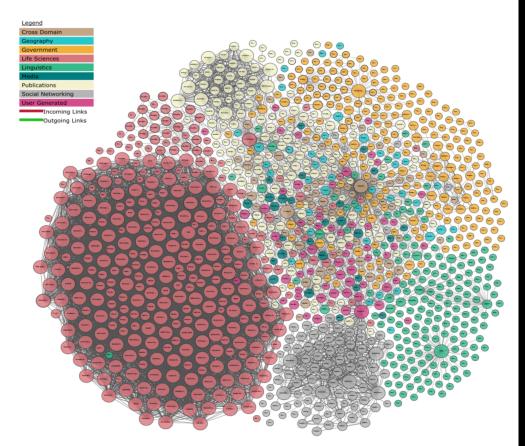
Linked Open Data (LOD)

FAIR Principles

Linked Data - Datasets under an open access

- 1,139 datasets
- over 100B triples
- about 500M links
- several domains

Gene Ontology: 807473 triples Lipid Ontology: 15406 triples

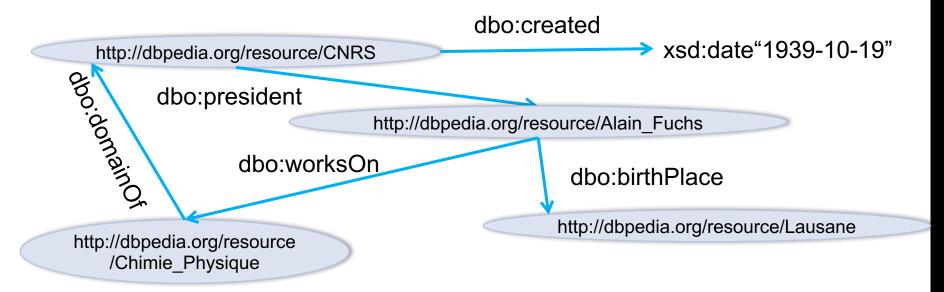


"Linking Open Data cloud diagram 2017, by Andrejs Abele, John P. McCrae, Paul Buitelaar, Anja Jentzsch and Richard Cyganiak. http://lod-cloud.net/"



RDF – RESOURCE DESCRIPTION FRAMEWORK

- An RDF Graph is a set of triples.
 - Its nodes are (labelled by) the subjects and objects appearing in the triples.
 - Its edges are labelled by the properties



NEED OF KNOWLEDGE

THE ROLE OF KNOWLEDGE IN AI

[Artificial Intelligence 47 (1991)]

ON THE THRESHOLDS OF KNOWLEDGE

Douglas B. Lenat

MCC 3500 W. Balcones Center Austin, TX 78759

Abstract

We articulate the three major fmdings of AI to date: (1) The Knowledge Principle: if a program is to perform complex task well, it must know a great deal about the world in which it operates. (2) A plausible extension of that principle, called the Breadth Hypothesis: there are two additional abilities necessary for intelligent behavior in unexpected situations: falling back on increasingly general knowledge, and analogizing to specific but far-flung knowledge. (3) AI as Empirical Inquiry: we must test our ideas experimentally, on large problems. Each of these three hypotheses proposes a particular threshold to cross, which leads to a qualitative change in emergent intelligence. Together, they determine a direction for future AI research. opponent is Castling.) Even in the case of having to search

Edward A. Feigenbaum

Computer Science Department

Stanford University Stanford, CA 94305

The knowledge principle: "if a program is to perform a complex task well, **it must know a great deal about the world** in which it operates."

there is some minimum knowledge needed for one to even formulate it.

SEMANTIC WEB: ONTOLOGIES

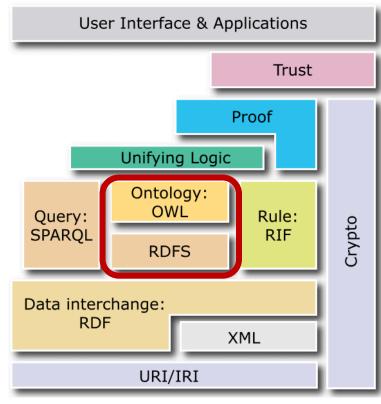
"An ontology is an **explicit**, **formal** specification of a shared conceptualization." [Thomas R. Gruber, 1993]

RDFS – Resource Description Framework Schema

Lightweight ontologies

OWL – Web Ontology Language

Expressive ontologies



Source: <u>https://it.wikipedia.org/wiki/File:W3C-</u> Semantic Web layerCake.png

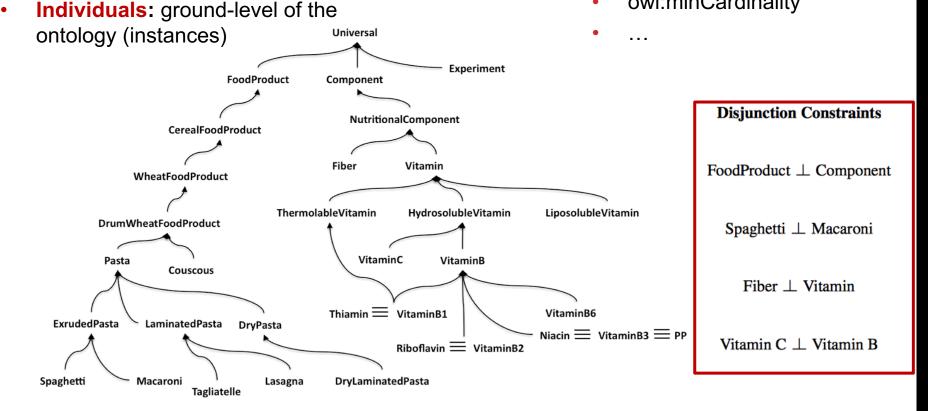
OWL – WEB ONTOLOGY LANGUAGE

- **Classes:** concepts or collections of • objects (individuals)
- **Properties:**

•

- owl:DataTypeProperty (attribute)
- owl:ObjectProperty (relation)

- Axioms
 - owl:subClassOf
 - owl:subPropertyOf •
 - owl:inverseProperty
 - owl:FunctionalProperty •
 - owl:minCardinality



KNOWLEDGE GRAPHS

WHO IS DEVELOPING KNOWLEDGE GRAPHS?



Academic side

WHO IS DEVELOPING KNOWLEDGE GRAPHS?

2007





Here the second second



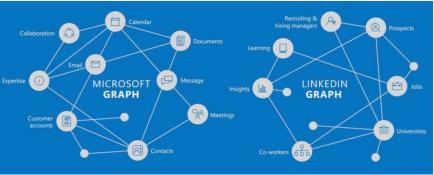
²⁰⁰⁷ Freebase

2012 Google Knowledge Graph

2015

2016

2013





Commercial side

Academic side

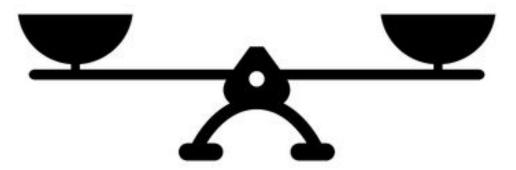
KNOWLEDGE GRAPH REFINEMENT

Completeness Correctness

KNOWLEDGE GRAPH REFINEMENT

Completeness

Correctness



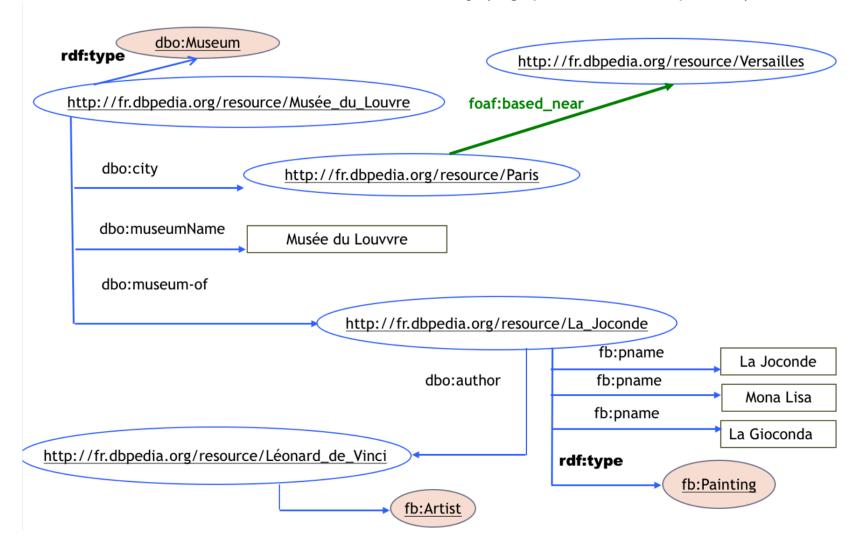
Data Linking Key discovery Data Fusion Link Invalidation Contextual identity

OUTLINE

- Introduction
- Key discovery for data linking
- Link Invalidation
- Contextual identity
- Conclusion

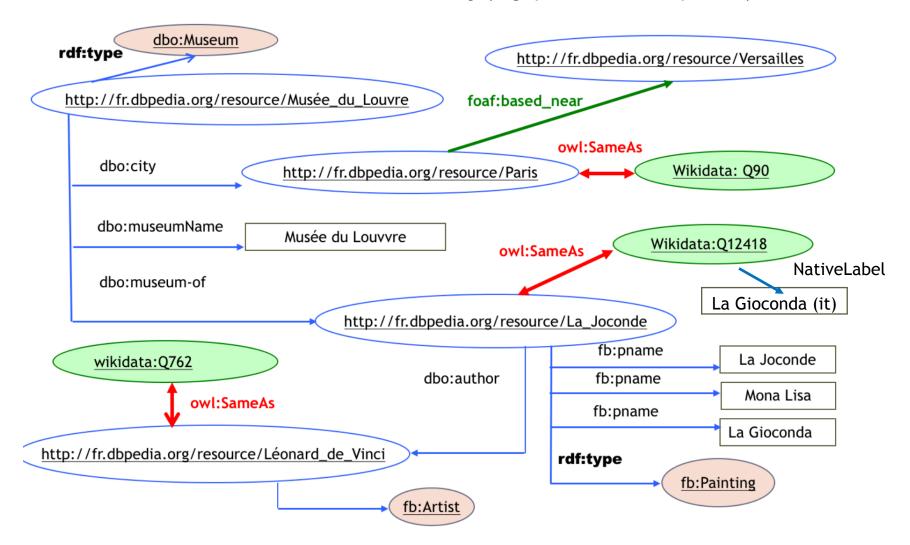
DATA LINKING

Data linking or Identity link detection consists in detecting whether two descriptions of resources refer to the same real world entity (e.g. person, article, protein).



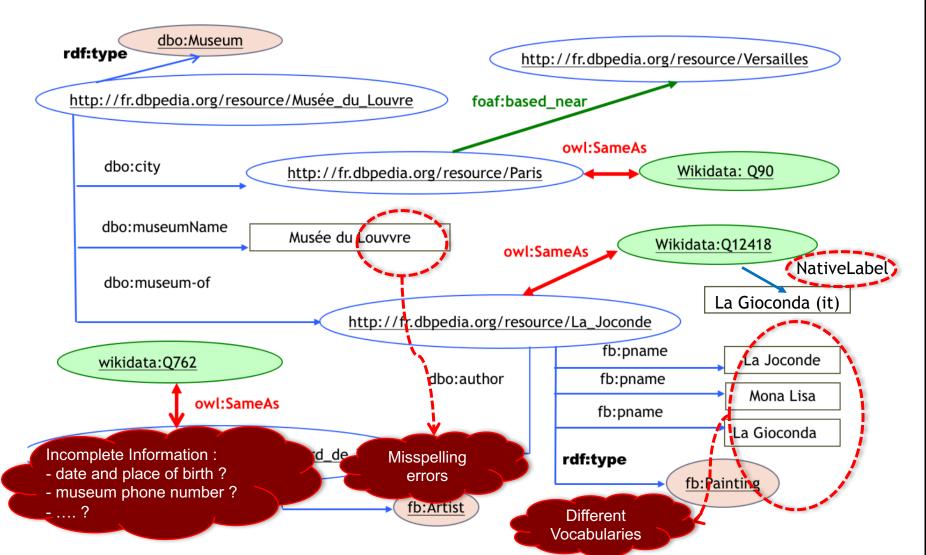
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DATA LINKING APPROACHES

• Local approaches: consider properties to compare pairs of instances independently

versus

- Global approaches: consider data type properties (attributes) as well as object properties (relations) to propagate similarity scores/linking decisions (collective data linking)
- **Supervised approaches**: need samples of linked data to learn models, or need interactions with expert

versus

- **Informed approaches**: need knowledge to be declared in the ontology or in other format
- Some surveys:
 - 1. Alfio Ferrara, Andriy Nikolov, François Scharffe:Data Linking. J. Web Semant. 23: 1 (2013)
 - 2. Markus Nentwig, Michael Hartung, Axel-Cyrille Ngonga Ngomo, Erhard Rahm: A survey of current Link Discovery frameworks. Semantic Web 8(3): 419-436 (2017)

KNOWLEDGE-BASED DATA LINKING

Rule-based data linking approaches [Saïs et al. 2009, Al Bakri et al. 2015]: need for knowledge to be declared in an ontology language or other languages.

```
homepage(X, Y) \land homepage(Z, Y) \rightarrow sameAs(X, Z)
```

Then we may infer:

sameAs(museum11, museum21)
sameAs(museum12, museum22)
sameAs(museum13, museum23)

	 homepage		SamaAa		homepage	
museum11	www.louvre.com	←	SameAs	→	www.louvre.com	museum21
museum12	www.musee-orsay.fr	÷	SameAs	→	www.musee-orsay.fr	museum22
museum13	www.quai-branly.fr	4	SameAs	→	www.quai-branly.fr	museum23
museum14						museum24

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A key: is a set of properties that uniquely identifies every instance of a class

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How to automatically discover keys from KGs?

KEY VALIDITY: KEYS WITH EXCEPTIONS

A key is a set of properties that uniquely identifies every instance in the

data

	FirstName	LastName	City	Profession	
Person1	Anne	Tompson	Paris	Actor, Director	
Person2	Marie	Tompson	Berlin	Actor	
Person3	Marie	David	Toulouse	Actor	
Person4	Vincent	Solgar	Rome	Actor, Director	
Person4	Simon	Roche	Montpellier	Teacher	
Person4	Jane	Ser	Paris	Teacher, Researcher	
Person4	Sara Khan		London	Teacher	
Person4	Theo	Martin	Lyon	Teacher, Researcher	
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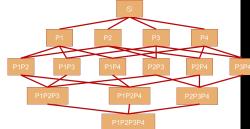
Is [FirstName,LastName] a key? ✓ Is [City] a key? ¥ Is [City] a key with 2 exceptions? ✓





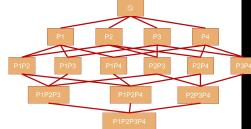
KEY DISCOVERY: A COMPLEX PROBLEM

- Find all the minimal keys requires at least 2ⁿ property combinations
 - need of efficient filtering and prunings



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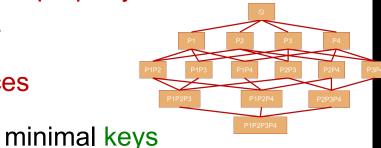
Find all the minimal keys requires at least 2ⁿ property combinations need of efficient filtering and prunings

derive

- For each combination scan all the instances
 - maximal non-keys \geq

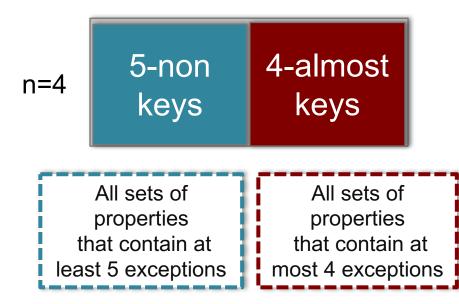
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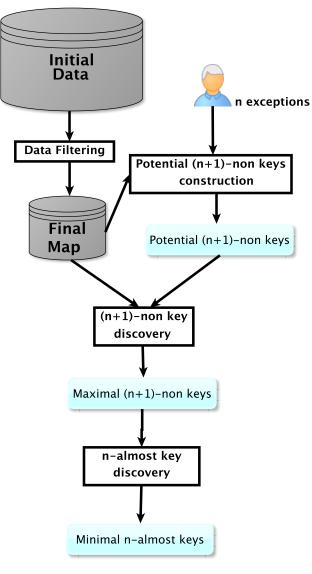




SAKEY: N-ALMOST KEY DISCOVERY

- SAKey allows *n* exceptions in the data
- n-almost key: a set of properties where |E_P|≤ n
- n-non key: a set of properties where |E_P|≥ n+1





APPLICATION TO SCIENTIFIC DATA

Many scientific numerical data

- Sensor data
- Experimental data..
- Difficult to interpret numerical data
 - Different levels of precision
 - Different measure units...
- Better understand the numerical data



Danai Symeonidou, Isabelle Sanchez, Madalina Croitoru, Pascal Neveu, Nathalie Pernelle, Fatiha Saïs, Aurelie Roland-Vialaret, Patrice Buche, Aunur-Rofiq Muljarto, Remi Schneider:Key Discovery for Numerical Data: Application to Oenological Practices. ICCS 2016: 222-236

APPLICATION TO SCIENTIFIC DATA

Discover keys in numerical data

• Keys: combinations of properties that discriminate a resource

Evaluate their quality

• Experimental numerical data in 3 wine flavour datasets (2011-2014)



How do we discriminate the wines??

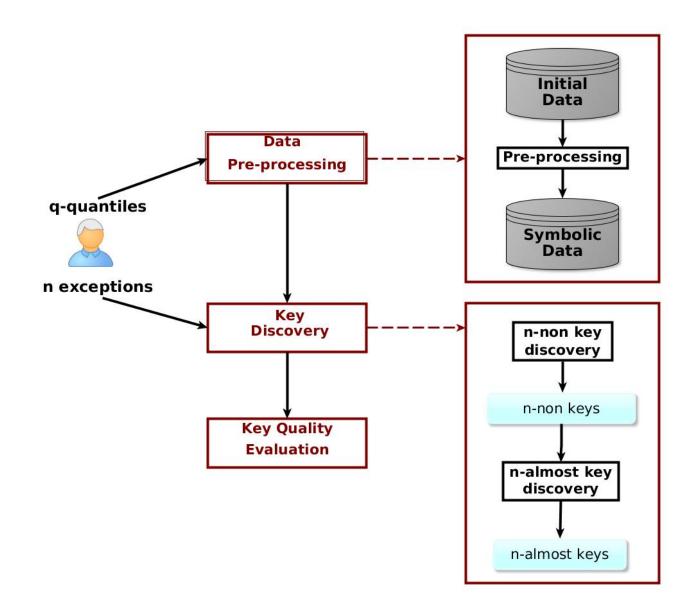
PROBLEM STATEMENT

Key discovery approaches consider all the values as symbolic

Ex. PH(Wine1, 3.455), PH(Wine2, 3.457)

Key discovery in raw numerical data: Many not-significant keys can be found

PROPOSED METHOD STEPS

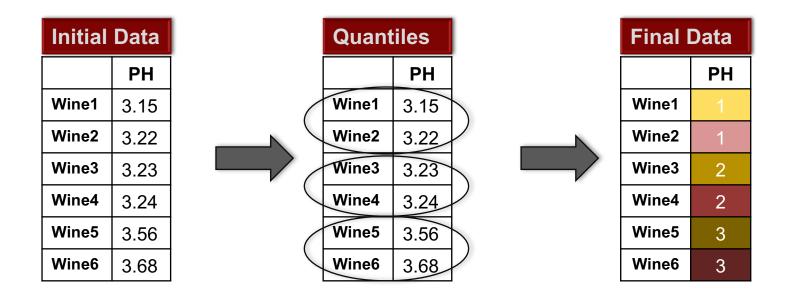


DATA PRE-PROCESSING

Objective: Interpret numerical data in a symbolic way

Solution: Use *quantiles* to group data values

- Quantiles: Cut points dividing a set of observations into equal-sized groups
 - Many quantiles → Discovery of false keys
 - Few quantiles → Lose of true keys



KEY QUALITY MEASURES

- 1) Key support
 - Intuition: The higher is the support the more sure is a key
- 2) Key exceptions
 - Intuition: A 0-almost key is considered more reliable than a 10-almost key
- 3) Key size
 - Intuition: Keys composed of few properties are preferred (easier to interpret)
- 4) Property correlation: The dependence of properties co-appearing in a key
 - Intuition: The less correlated are the properties participating in a key, the more informative the key is

EXPERIMENTAL DATA

Chemical families	Concentration levels in wine	Analyzed molecules	Analysis methodology
Thiols	ppt	3MH = 3 mercaptohexanol	LC-MS/MS
		3MHA = 3 mercaptohexylacetate	
Esters	ppm	2PHEN= 2-phenylethanol	GC-MS/MS
		AH= hexyl acetate	
		AI= isoamyl acetate	
		ABPE= phenethyl acetate	
		DE= ethyl decanoate	
		HE= ethyl hexanoate	
		OE= ethyl octanoate	
		BE= ethyl butyrate	
		2HPE= Ethyl lactate	
		3HBE= Ethyl 3-hydroxybutyrate	
		2MBE= Ethyl 2-methylbutyrate	
		2MPE= Ethyl isobutyrate	
		2HICE= Ethyl leucate	
C13-	Ppb	BDAM= beta-damascenone	GC-MS/MS
noriprenoïds		BION= beta-ionone	
PDMS	Ppb	Dimethylsulfide potential= S-methylmethione +	GC-MS/MS
		others compounds	
GSH	ppm	Glutathione	LC-MS/MS

EXAMPLES OF KEYS

	Year	Quantiles	Support	Probability	Size
[3MHA, BDAM, GSH, 2MPE, 3MH]	2014	5	73%	26%	5
[3MHA, GSH, OE, 2HICE, 3MH]	2014	5	73%	26%	5
[3MHA, AI, PDMS, 2MPE, 3MH]	2014	5	100%	26%	5
[3MHA, BE, PDMS, 2MPE, 3MH]	2014	5	100%	26%	5
[BDAM, OE, PDMS, 3MH]	2012	10	100%	17%	4
[GSH, OE, PDMS, 2PHEN]	2012	10	100%	17%	4
[AI, BDAM, 2HICE, 3MH]	2012	10	100%	17%	4
[3MHA, BDAM, GSH, 2MPE]	2013	5	63%	94%	4
[3MHA, BDAM, GSH]	2013	12	63%	64%	3
[AH, BDAM, GSH]	2013	12	63%	64%	3
[BE, 2HICE, 3MH]	2013	12	100%	64%	3
[BDAM, GSH, 3MH]	2013	12	63%	63%	3
[GSH, PDMS, 3HBE]	2013	10	63%	83%	3
[BDAM, GSH, 3MH]	2013	10	63%	83%	3
[GSH, PDMS, 3HBE]	2014	10	73%	63%	3
[PDMS, 3HBE, 3MH]	2014	12	100%	44%	3
[3MHA, GSH, PDMS]	2014	12	73%	44%	3
[BE, GSH, 3MH]	2014	12	73%	44%	3

VALIDATED KEYS

- 18 out of 104 keys (18%) were validated by the expert
- Support from 63% to 100%
 - Keys with low support can be as well significant
- Evaluated keys contain from 3 to 5 properties
 - Expert chose keys with big size (on contrary to the initial intuition)
- Example: Key {AI, BDAM, 2HICE, 3MH}
 - Correlations from 0.05 to 0.42
 - Properties not highly correlated → interesting keys
- First step for predicting wine taste and wine component concentration

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OAEI*: RECENT RESULTS

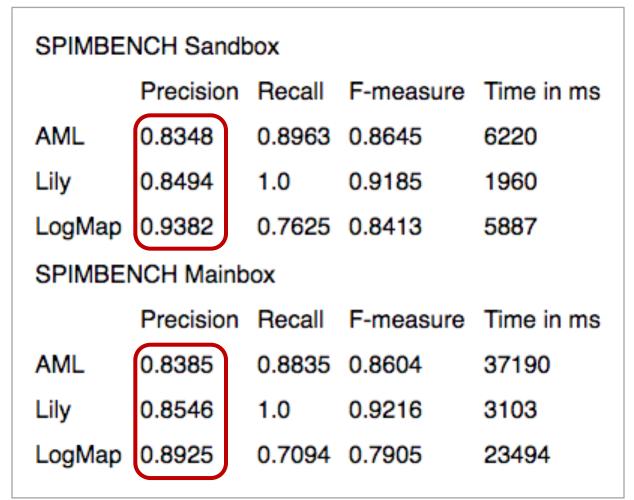
• Data Linking results for OAEI 2018 - SPIMBENCH Track

SPIMBENCH Sandbox				
	Precision	Recall	F-measure	Time in ms
AML	0.8348	0.8963	0.8645	6220
Lily	0.8494	1.0	0.9185	1960
LogMap	0.9382	0.7625	0.8413	5887
SPIMBE	SPIMBENCH Mainbox			
	Precision	Recall	F-measure	Time in ms
AML	0.8385	0.8835	0.8604	37190
Lily	0.8546	1.0	0.9216	3103
LogMap	0.8925	0.7094	0.7905	23494

* OAEI: Ontology Alignment Evaluation Initiative

OAEI*: RECENT RESULTS

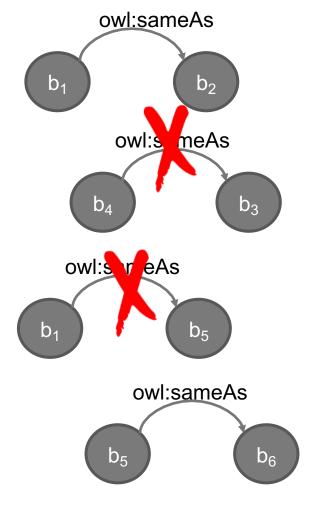
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IDENTITY PROBLEM

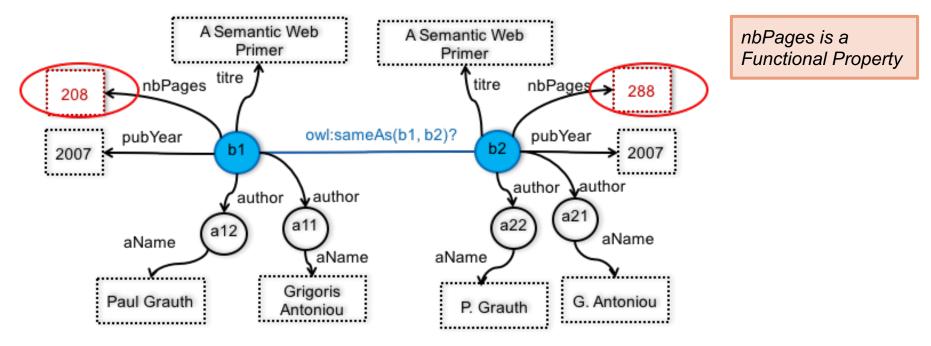
- In [Jaffri et al., 2008], the authors discuss how erroneous use of owl:sameAs in the interlinking of the DBpedia and DBLP datasets has resulted in publications becoming incorrectly assigned to different authors.
- [Halpin et al. 2010] showed that 37% of owl:sameAs links randomly selected among 250 identity links between books were incorrect.
- Automatic data linking tools do not guarantee 100% precision, because of:
 - Errors, missing information, data freshness, etc.



IDENTITY LINK INVALIDATION

[Papaleo et al., 2014]

Principle: use of ontology axioms (functionality, local completeness, asymmetry, etc.) to detect inconsistencies or error candidates in the linked resources descriptions.

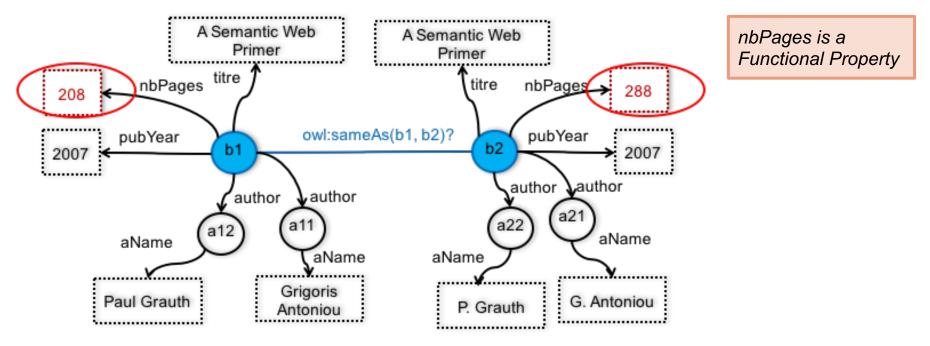


Laura Papaleo, Nathalie Pernelle, Fatiha Saïs, Cyril Dumont:Logical Detection of Invalid SameAs Statements in RDF Data. EKAW 2014: 373-384

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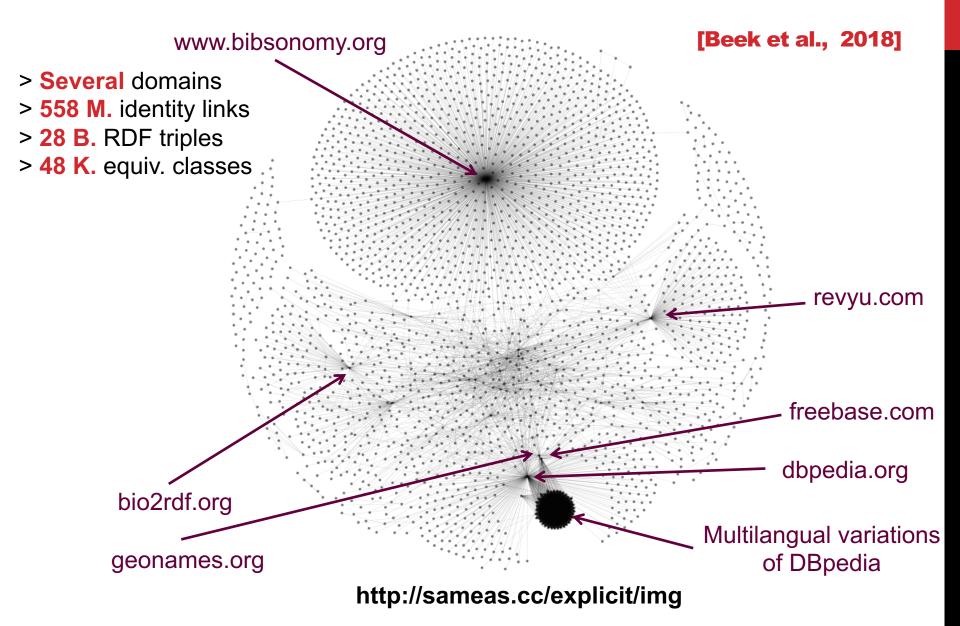


Improvements in data linking precision up to 25%

Limits:

• Scalability problems and need of uniform vocabulary in datasets

IDENTITY PROBLEM AT LOD SCALE



IDENTITY PROBLEM AT LOD SCALE

[Beek et al., 2018]

← → C 🗎 Secure | https://sameas.cc/term?page=1&page_size=20&id=4073

SameAs.cc Documentation Identity sets Terms Triples

Terms for identity set 4073

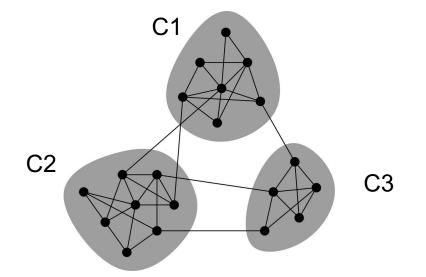
- <http://af.dbpedia.org/resource/%D0%A7> (→ id) 〈s, owl:sameAs, o〉
- <http://af.dbpedia.org/resource/%D1%A4> (→ id) (s, owl:sameAs, o)
- <http://af.dbpedia.org/resource/7> (→ id) 〈s, owl:sameAs, o〉
- <http://af.dbpedia.org/resource/Aandelebeurs> (→ id) 〈s, ow1: sameAs, o〉
- <http://af.dbpedia.org/resource/Afghanistan> (↦ id) 〈s, owl:sameAs, o〉
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- <http://af.dbpedia.org/resource/Albany,_New_York> (→ id) 〈s, owl:sameAs, o〉
- <http://af.dbpedia.org/resource/Albert_Einstein> (↦ id) ⟨s, owl:sameAs, o⟩
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- <http://af.dbpedia.org/resource/Amerikaanse_Maagde-eilande> (↦ id) 〈s, owl:sameAs, o〉
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- <http://af.dbpedia.org/resource/Andorra_la_Vella> (↦ id) 〈s, owl:sameAs, o〉
- <http://af.dbpedia.org/resource/Angola> (→ id) 〈s, owl:sameAs, o〉
- <http://af.dbpedia.org/resource/Anguilla_(eiland)> (→ id) 〈s, owl:sameAs, o〉

The largest identity set contains 177 794 terms:

Different countries Different cities Albert Enstein

 \rightarrow quality problems

[Raad et al., ISWC 2018]



- Considers the identity network build from the explicit identity network of sameAs links: removing of symmetric and reflexive links.
- Uses of Louvain community detection algorithm to detect subgraphs in the identity network that are highly connected.
- Defines a ranking score for each (intra-community and inter-community) identity link based on the density of the community.

Joe Raad, Wouter Beek, Frank van Harmelen, Nathalie Pernelle, Fatiha Saïs:Detecting Erroneous Identity Links on the Web Using Network Metrics. International Semantic Web Conference (1) 2018: 391-407

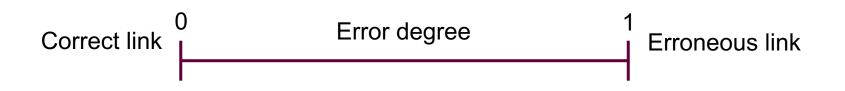
Ranking of identity links

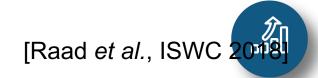
intra-community erroneousness degree

a)
$$err(e_C) = \frac{1}{w(e_C)} \times \left(1 - \frac{W_C}{|C| \times (|C| - 1)}\right)$$

inter-community erroneousness degree

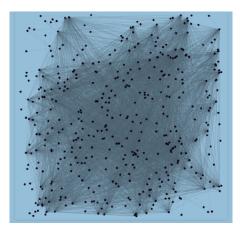
b)
$$err(e_{C_{ij}}) = \frac{1}{w(e_{C_{ij}})} \times \left(1 - \frac{W_{C_{ij}}}{2 \times |C_i| \times |C_j|}\right)$$



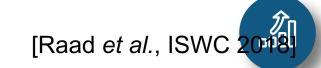


Dataset

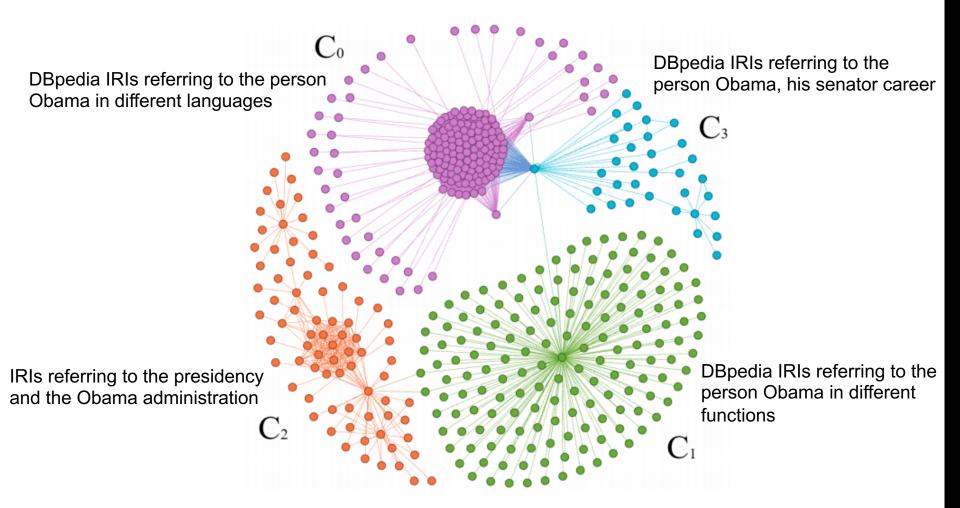
- LOD-a-lot dataset [Fernandez et al. 2017]: a compressed data file of 28B triples from LOD 2015 crawl
- An explicit identity network of 558.9M edges (links) and 179M nodes (resources)

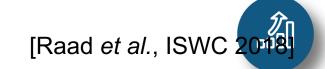


Example: The *B*. *Obama* equality set that contain 440 nodes

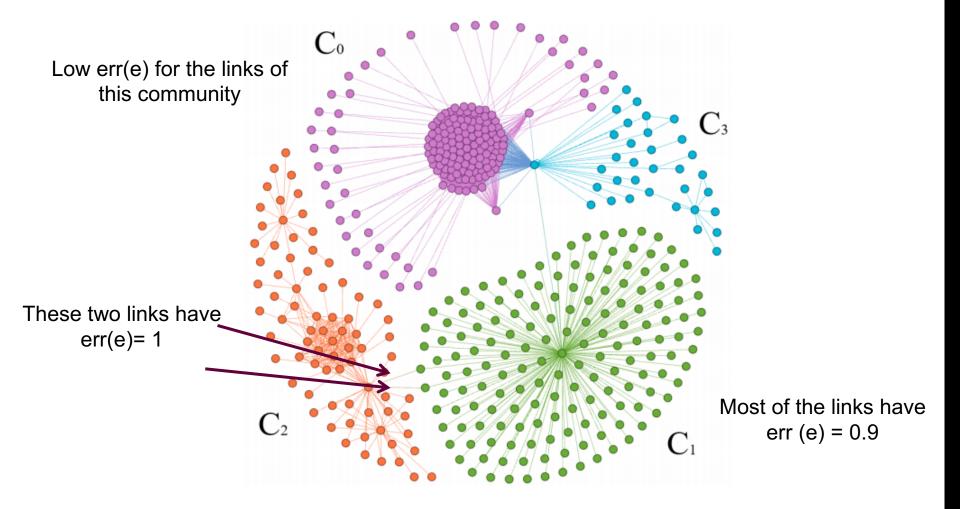


Barack Obama's Equality Set





Barack Obama's Equality Set



LINK INVALIDATION: NETWORK-BASED APPROACH EVALUATION [Raad et al. 2018]

• Scales to a graph of 28 billion triples: 11 hours for the 4 steps

No **benchmark** for qualitative evaluation

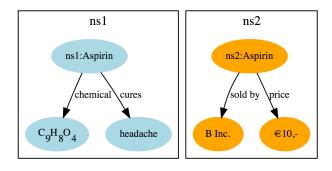
Precision: manual evaluation of 200 links

- The higher the error degree is the most likely the link will be erroneous: 100% of owl:sameAs with an error degree <0.4 are correct</p>
- Can theoretically invalidate a large set of owl:sameAs links on the LOD:
 1.26M owl:sameAs have an error degree in [0.99, 1]

Recall:780 incorrect linksbetween 40 distinct resources have beenintroduced in the explicit identity graph.Recall = 93 %

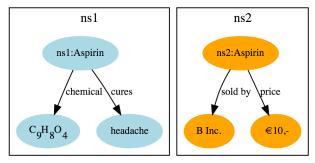
SOMETIMES, WE NEED WEAKER IDENTITY ...

- Identity is context-dependent [Geach, 1967]
 - allowing two medicines to be considered the same in terms of their chemical substance, but different in terms of their price

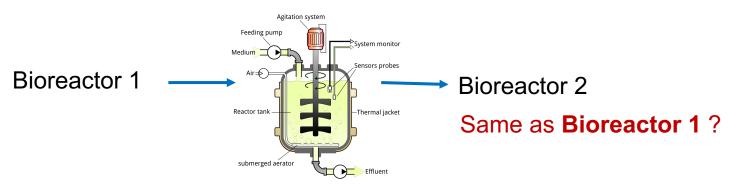


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- Identity over time poses problems
 - a material could it be considered the same, even though some (or even all) of its original components have been replaced by new ones.



OWL:SAMEAS PREDICATE IS TOO STRICT

- owl:sameAs, indicates that two different descriptions refer to the same entity
- a strict semantics,
 - 1) Reflexive,
 - 2) Symmetric,
 - 3) Transitive and
 - 4) Fulfils property sharing:

 $\forall X \forall Y \text{ owl:sameAs}(X, Y) \land p(X, Z) \Rightarrow p(Y, Z)$

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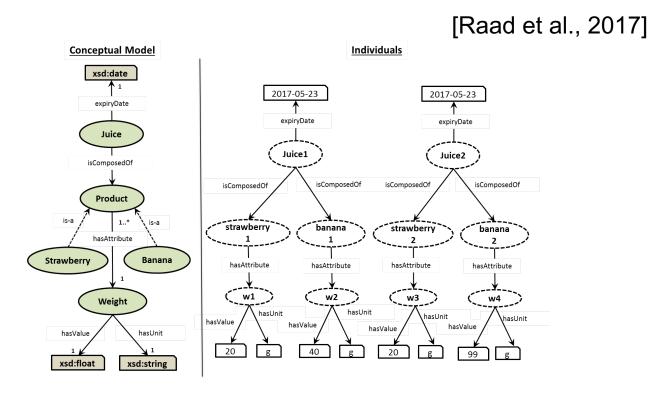
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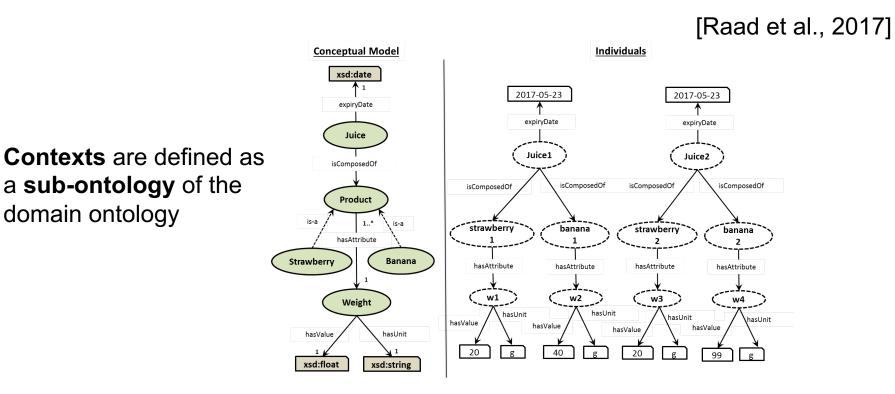
Detection of weak-identity links -> Contextual Identity

[Raad et al., 2017]

- New predicate :<u>identiConTo</u> for expressing contextual identity relation
- An algorithm for automatic detection of the most specific contexts in which two instances (resources) are identical
 - the detection process can further be guided by a set of semantic constraints that are provided by domain experts.
- Contexts are defined as a sub-ontology of the domain ontology

Joe Raad, Nathalie Pernelle, Fatiha Saïs: Detection of Contextual Identity Links in a Knowledge Base. K-CAP 2017: 8:1-8:8





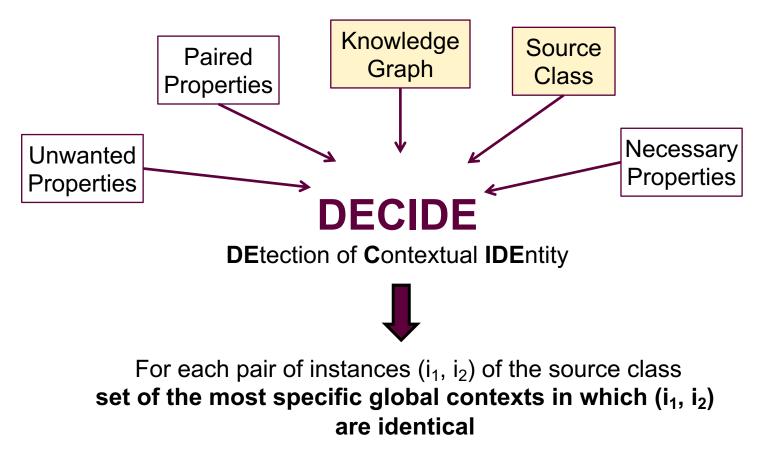
Contextual Identity Link Example

Π_a(Juice) = { (Juice, {rdf:Type, expiryDate}, {isComposedOf}), (Banana, {rdf:Type}, {isComposedOf ⁻¹}), (Strawberry, {rdf:Type}, {hasAttribute, isComposedOf ⁻¹}), (Weight, {rdf:Type, hasValue, hasUnit}, {hasAttribute⁻¹}) }

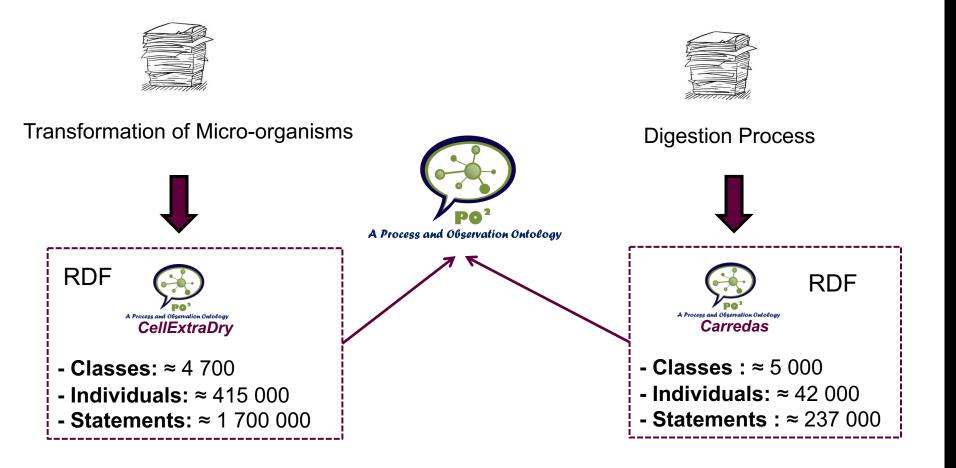
identiConTo<(Tailor))</pre>(juice1, juice2)

[Raad et al., 2017]

It automatically detects and adds these contextual identity links in the knowledge graph

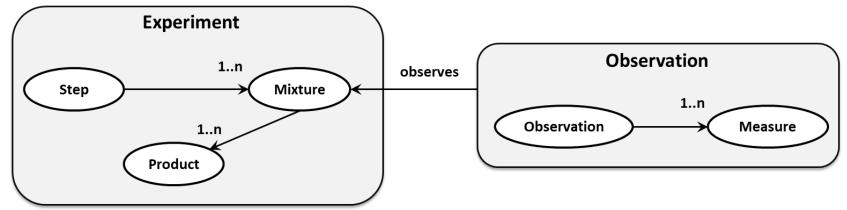


LIONES*: CONTEXTUAL IDENTITY LINKS [Raad et al., 2017]



* LIONES project funded by CDS Paris Saclay (2015-2018)





Detect for each context **GC**_i, the measures **m**_i where

 $\label{eq:identiConTo_{GCi}} \begin{array}{l} (i_1,\,i_2) \cap \textit{observes}(i_1,\,m_1) \rightarrow \textit{observes}(i_2,\,m_2) \\ & \text{with } m_1 \simeq m_2 \end{array}$

 $identiConTo_{<GCi>}(i1, i2) \rightarrow same(m_i)$



Detection of 38 844 rules

Règle	Taux d'erreur	Support
$identiConTo_{}(x, y) \\ \rightarrow same(pH)$	6.19 %	57
$identiConTo_{}(x, y) \\ \rightarrow same(Dureté)$	1.86 %	66
	4.52 %	647

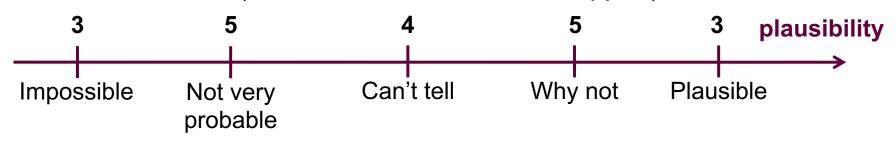
The domain experts has evaluated the plausibility of the best **20 rules** (in termes of error rate and support)



Detection of 38 844 rules

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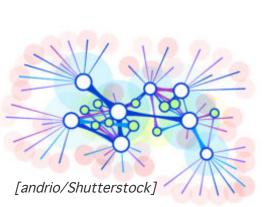
The error rate decreases of 12% when a global context is replaced by a more specific global context

WARM RULES – GRADUAL CAUSAL RULES DETECTION IN KNOWLEDGE GRAPHS

Application to plant development in climatic warming preoccupation

Phenology: the study of seasonal cycles of plants (timing and duration of flowering, fruiting, leaf out and leaf drop)

VE VI V3 V6 V9 VT VE VI V3 V6 V9 VT Sensor Measurement Forecast Expert Knowledge and Observations



Domain-specific Knowledge Graphs



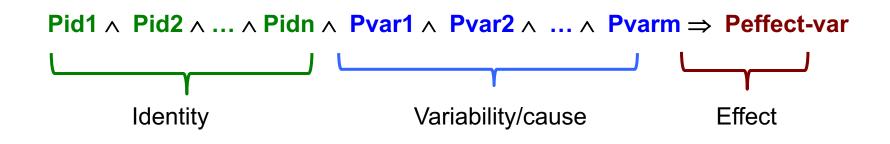


MIA/INRA

GQE

LRI/UPS

GRADUAL CAUSALITY RULE DATAIA DISCOVERY IN RDF KGS



Example:

Humidity(X,h1):t1 Humidity(Y,h2):t2

(h1> h2) \land (temp1 < temp2) \land (t1< t2) \Rightarrow flowering-delay(Y)

CONCLUSION

- Semantic Web standards, agronomic data/knowledge and many applications are there
- Promising applications are emerging for which reasoning on data is central:
 - Information retrieval, decision-support, digital-assistants, ...
- Many challenges remain to handle at large scale the incomplete, uncretain and evolving knowledge graphs
 - Combining numerical and symbolic AI is challenging but worthwhile to investigate more deeply.

DATA LINKING AND KNOWLEDGE DISCOVERY IN RDF DATA: METHODS AND SOME FEEDBACK FROM AGRONOMIC APPLICATIONS

FATIHA SAÏS



LAHDAK@LRI, PARIS SUD UNIVERSITY, CNRS, PARIS SACLAY UNIVERSITY

Joint work with: N. Pernelle, L. Papaleo, J. Raad and D. Symeonidou

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KEY QUALITY MEASURES

Non-key probability: The probability that a set of properties contains instances sharing the same values for this set

$$Pr_k = 1 - e^{-\frac{n(n-1)}{2p}}$$

with
$$p = \Pi_{i=0}^{j} m_{i}$$
 where

j:# of properties
m_i:# of distinct values

KEY QUALITY MEASURES

Non-key probability

Example: 100 distinct wines

	Case1	Case2	Case3
WineName	15 distinct values	50 distinct values	90 distinct values
YearProduction	10 distinct values	50 distinct values	80 distinct values
Non-key probability	1	0.87	0.49

 Intuition: Higher is the non-key probability of {wineName, yearProduction}

more the discovered key is important

EXPERIMENTS

Experimental data: 3 wine aroma datasets

- Different chemical based flavourings of wine
 - Concentration of each flavour in a wine

	# Instances	# Flavours
D1 (2011 – 2012)	63	19
D2 (2012 – 2013)	59	19
D3 (2013 – 2014)	44	19

Goal: Verify the interest of keys in numerical data

- Evaluate the impact of quantiles in the results
- Evaluate the quality measures

DATA PREPROCESSING

Quantiles

Use the non-key probability to define the number of quantiles

5, 10, 12 quantiles

- Setting it at less than 5 => no keys are obtained
- Using 5 to 12 quantiles ensured a significantly high probability