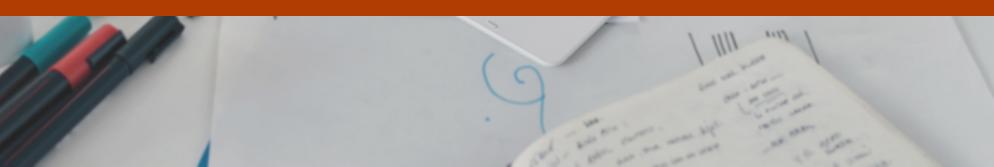
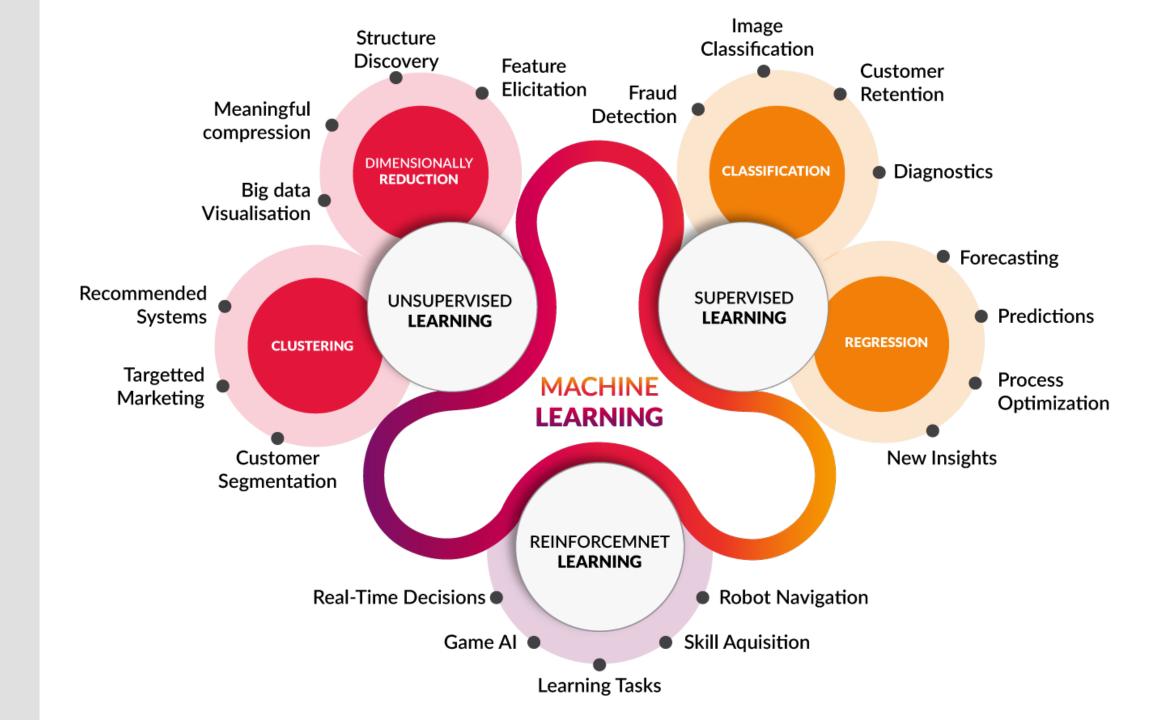
# ONTOLOGY DRIVEN MACHINE LEARNING -- Nguyen Hung Son --



# The Lecture Outline

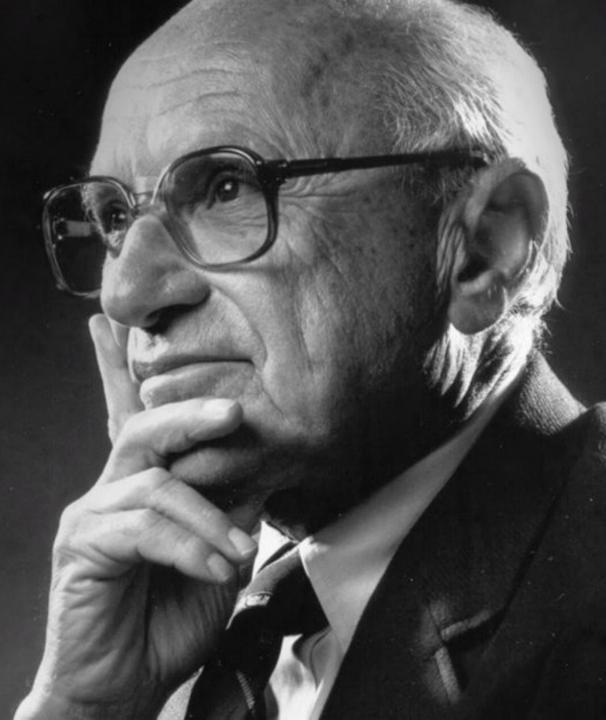
- Domain Knowledge in Machine Learning
- Knowledge representation methods: ontology, taxonomy, ...
- Ontology driven machine learning
  - Ontology and classification
  - Ontology and clustering
  - Semantic evaluation of clustering algorithms
  - Semantic search and text mining
- Machine learning and knowledge acquisition
- Concluding remarks



# Domain knowledge in Machine learning

lilton Friedman favorite political aphorism:

# "There's no such thing as a free lunch."



# No free lunch theorem

• Assume  $\mathcal{A}$  is a searching algorithm that looking for the maximum of a function  $f: S \rightarrow W$ 

where S is a finite set of states, W is a finite subset of **R**, and  $f \in \mathcal{F}$ 

- The work of algorithm **A** after *t* steps can be identified by the sequence:  $V_{\mathcal{A}}(f,t) = \left[ (s_1, f(s_1)), (s_2, f(s_2)), ..., (s_t, f(s_t)) \right]$
- The quality of algorithm  $\mathcal{A}$  can be measured by an evaluation function:  $M:\{V_{\mathcal{A}}(f,t)|\mathcal{A},f,t\} o\mathbb{R}$
- for example:  $M(V_A(f,t)) = \min\{i|f(s_i) = f_{\max}\}$

# No free lunch theorem

• The class  $\mathcal{F}$  satisfies NFL condition: if the following equation

$$\sum_{f\in\mathcal{F}} M(V_\mathcal{A}(f,|S|)) = \sum_{f\in\mathcal{F}} M(V_{\mathcal{A}'}(f,|S|))$$

holds for any measure M and any pair of algorithms  $\mathcal{A}, \mathcal{A}'$ 

•  $\mathcal{F}$  is closed under permutation: for any permutation  $\sigma \in Perm(S)$ and  $f \in \mathcal{F}$  we have  $\sigma f \in \mathcal{F}$ 

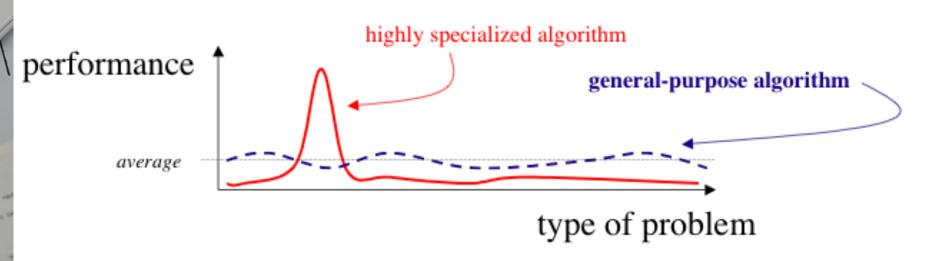
#### NFL theorem:

the class  $\mathcal{F}$  satisfies NFL condition iff  $\mathcal{F}$  is closed under permutation

# No free lunch

- For example: the class of all functions from *S* to *W* is closed under permutation
- The probability that a random class of functions from *S* to *W* is closed under permutation equals O(|S|+|W|-1)

$$rac{2^{inom{|S|+|W|-1}{|S|}}-1}{2^{|S|^{|W|}}-1}$$



# No free lunch theorem for learning

Wolpert (1996) shows that in a noise-free scenario where the loss function is the misclassification rate, if one is interested in off-training-set error, then there are no a priori distinctions between learning algorithms.

More formally, where

- d = training set;
- m = number of elements in training set;
- f = 'target' input-output relationships;
- h = hypothesis (the algorithm's guess for f made in response to d); and
- C = off-training-set 'loss' associated with f and h ('generalization error')
- all algorithms are equivalent, on average, by any of the following measures of risk: E(C|d), E(C|m), E(C|f,d), or E(C|f,m).

# Therefore ...

- No search or learning algorithm can be the best on all possible learning or optimization problems.
- In fact, every algorithm is the best algorithm for the same number of problems.
- But only some problems are of interest.
- For example:

a random search algorithm is perfect for a completely random problem (the ``white noise" problem), but for any search or optimization problem with structure, random search is not so good. KNOWLEDGE PRESENTATION METHODS: classification, taxonomy, ontology, thesaurus.

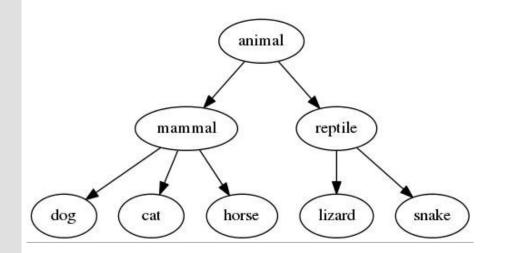
# Merriam-Webster definition

#### **Classification**

• systematic arrangement in groups or categories according to established criteria

#### Taxonomy

• orderly classification of plants and animals according to their presumed natural relationships.



#### Ontology

- Old: a branch of metaphysics concerned with the nature and relations of being or a particular theory about the nature of being or the kinds of existents.
- New: machine-readable set of definitions that create a taxonomy of classes and subclasses and relationships between them

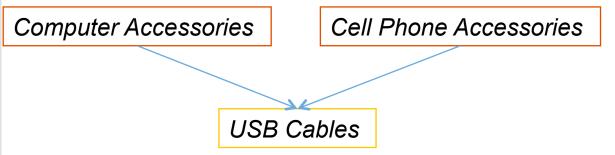
#### Thesaurus:

- *a thesaurus deals only with words, alternatives for those words, synonyms, translations, et cetera*
- *can be used by a classification, a taxonomy and an ontology*

# Ontology vs taxonomy

#### Taxonomy:

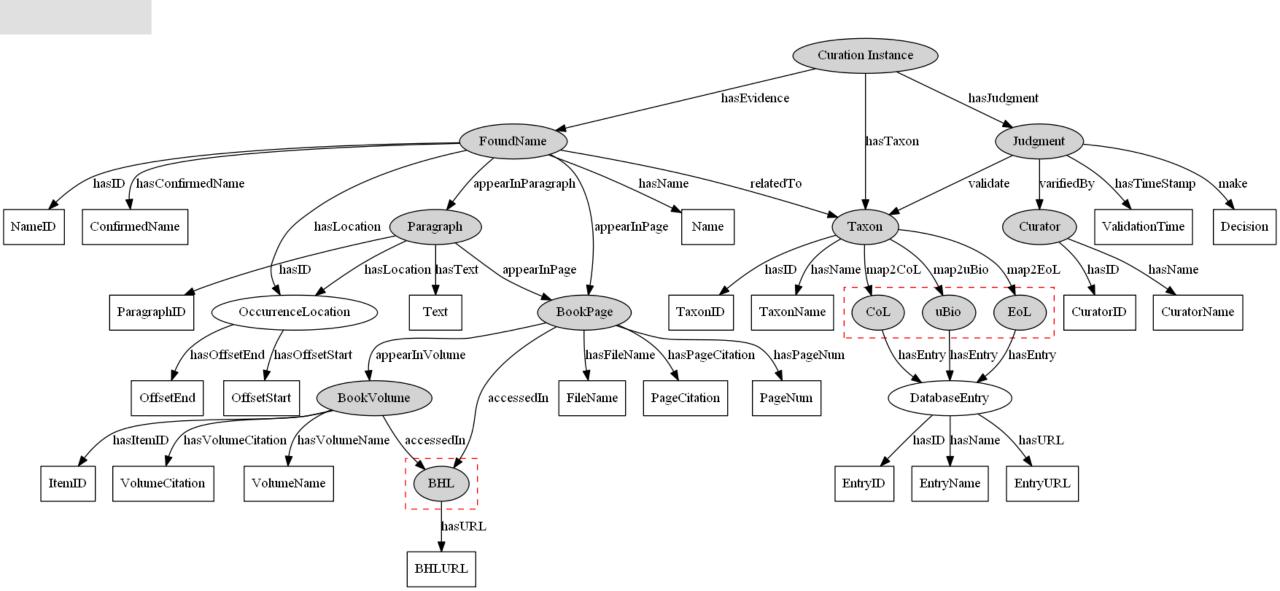
- Sub-concept relation only
- A proper taxonomy is a strict hierarchy (one parent), e.g.
  - Natural Science (500)
  - -> Zoological Sciences (590)
    - -> Other Invertebrates (595)
      - -> Insects (595.7)
        - -> *Lepidoptera (595.78)* 
          - -> Butterflies (595.789).
- Relaxed model: multi-parent but still noncyclic e.g.



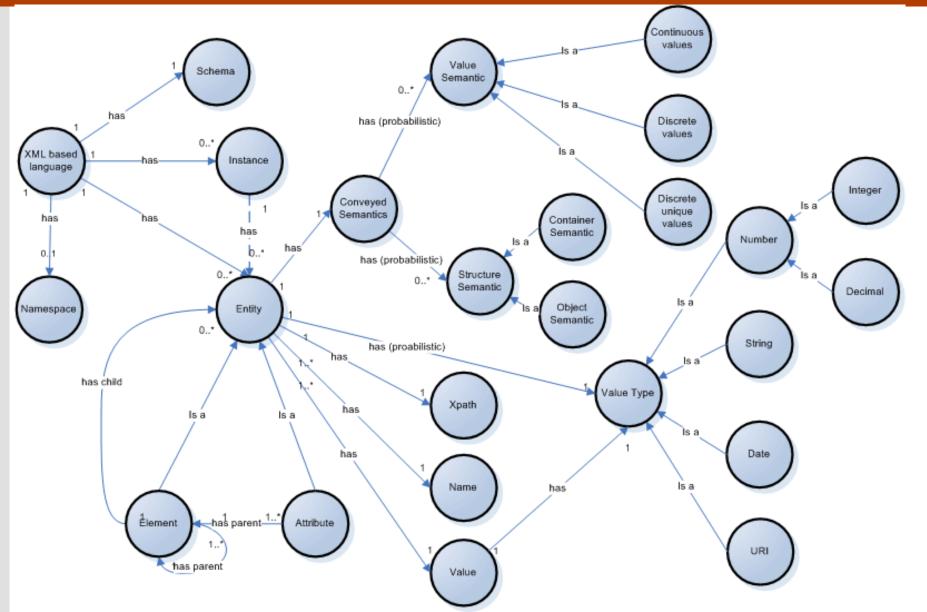
## Ontology

- Objects could be:
  - classes
  - instances of the class
  - class attributes
- More types of relations:
  - is-a
  - has-a
  - use-a
- the relationships aren't necessarily binary—for example, a co-worker

### Example of taxonomic name curation



# Example of XML entities ontology

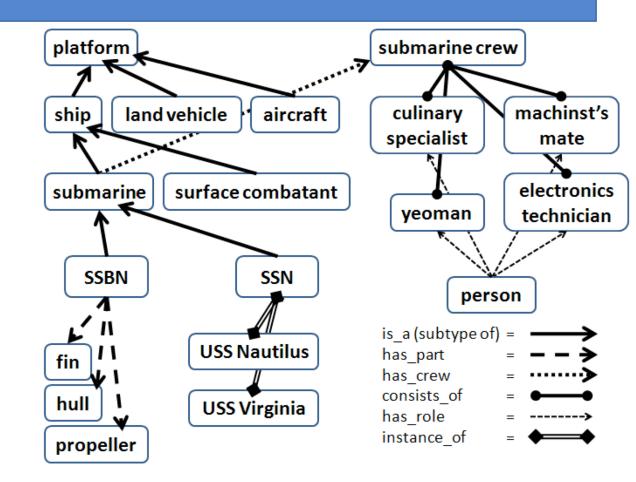


# What is ontology?

A structured, **taxonomic model** or representation of the **entities** and **relations** existing within a particular domain of reality.

For examples:

- Gene ontology,
- lexical ontology (wordnet),
- Ontology for General Medical Science
- other domain ontology



# **Ontology libraries & repositories**

#### LIBRARIES:

- A library system that offers various functions for managing, adapting and standardizing groups of ontologies.
- It should fulfill the needs for re-use of ontologies. In this sense, an ontology library system should be easily accessible and offer efficient support for reusing existing relevant ontologies and standardizing them based on upper-level ontologies and ontology representation languages.

#### **REPOSITORIES:**

- A structured collection of ontologies (...) by using an Ontology Metadata Vocabulary.
- References and relations between ontologies and their modules build the semantic model of an ontology repository. Access to resources is realized through semantically-enabled interfaces applicable for humans and machines.
- Therefore, a repository provides a formal query language.

Ontology libraries
OBO Foundry
WebProtégé
Romulus
DAML ontology library
Colore
VEST/AgroPortal Map of standards
FAIRsharing
DERI Vocabularies
OntologyDesignPatterns
SemanticWeb.org
W3C Good ontologies
TaxoBank
BARTOC
GFBio Terminology Service
agINFRA Linked Data Vocabularies
oeGOV
Ontology repositories
NCBO BioPortal*
Ontobee
EBI Ontology Lookup Service
AberOWL
CISMEF HeTOP
SIFR BioPortal*
OKFN Linked Open Vocabularies
ONKI Ontology Library Service
MMI Ontology Registry and Repository*

# Applications

#### **Vertical need**

- For those uses who want to do very precise things, e.g.
  - o reasoning,
  - o using specific relations
  - using only suitable ontologies (developed by the same communities and in the same format).
- For those users who may just use the repositories as libraries to find and download ontologies, and work in their own environment.

#### **Horizontal need**

- For those who wants to work with a wide range of ontologies and vocabularies useful in their domain but developed by different communities, overlapping and in different formats.
- Such users greatly appreciate the unique endpoints (Web application and programmatic for REST and SPARQL queries) offered by the repositories under a simplified common model.

# Ontology: challenges and applications

- Metadata & selection
- Multilingualism
- Ontology alignment
- Generic ontology-based services
- Annotations and Linked Data
- Scalability & interoperability

# Leslie Valiant

 A fundamental question for AI is to characterize the computational **building blocks** that are necessary for cognition.

- Turíng Award, 2010
- European Association for Theoretical Computer Science Award, 2008
- Knuth Príze, 1997
- Nevanlínna Príze, 1986



JANUARY 7, 2013 Computer scientist Leslie Valiant named 2012 ACM Fellow

- A specific challenge is to build on the success of machine learning so as to cover broader issues in intelligence.
- This requires, in particular a reconciliation between two contradictory characteristics
  - The apparent logical nature of reasoning and
  - the statistical nature of learning.
- Professor Valiant has developed a formal system, called robust logics, that aims to achieve such a reconciliation.

# Ontology driven methods for Machine Learning and AI

# Case studies

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- 1. Robocup
- 2. Semantic Text processing and mining
- 3. Approximate reasoning

# ROBOCUP: robocup.org

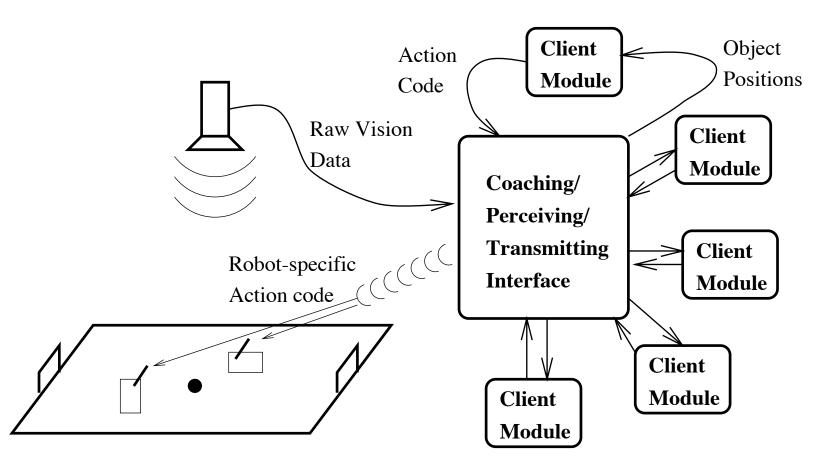
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HOME	ABOUT	ORGANIZATION	LEAGUES	EVENTS	NEWS	RESEARCH	GALLERY	INFO
RoboCup	Soccer - Sir	nulation				I	LEAGUES	
							Humanoid	
-	>		<u>t</u>				Standard Platfor	m
115	1		5				Middle Size	
-	1	33					Small Size	
			- AL	P			Simulation	
							SUB-LEAGUES	
		s in RoboCupSoccer. The					Simulation 2D	
	Independently m pleagues: 2D and	noving software players I 3D.	mputer.	Simulation 3D				

# robotic soccer architecture

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as a distributed deliberative and reactive system



# **Robocup and simulated robotic soccer**

#### Noda's Soccer Server

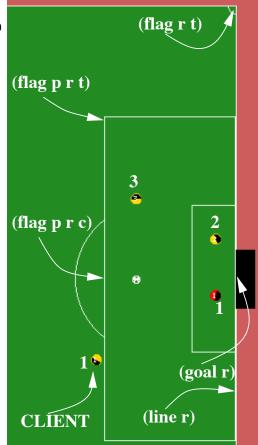
- the players' vision is limited (45°);
- the players can communicate by posting to a blackboard that is visible to all players;
- all players are controlled by separate processes;
- each player has 10 teammates and 11 opponents;
- each player has limited stamina;
- actions and sensors are noisy; and
- play occurs in real time.

The simulator, acting as a server, provides a domain and supports users who wish to build their own agents (clients).



## Example

```
(see 124 ((goal r) 20.1 34) ((flag r t) 47.5 -4) ((flag p r t) 30.3 -24) ((flag p r c) 10.1 -20)
((ball) 11 0) ((player usa 2) 21 19) ((player usa 3) 21 -11) ((player brazil 1) 17 35) ((line r) 40
**-> (dash 80)
(see 129 ((goal r) 16 43) ((flag r t) 42 -6) ((flag p r t) 25 -30) ((flag p r c) 5 -40) ((ball) 6 1)
((player usa 2) 16.3 24) ((player usa 3) 15.3 -17) ((line r) 32.8 -27))
**-> (turn 1)
**-> (dash 60)
(see 134 ((flag r t) 40 -9) ((flag p r t) 23.3 -35) ((ball) 3.7 2) ((player usa 2) 14.4 24)
((player usa 3) 13.3 -22) ((line r) 28.2 -30))
**-> (turn 2)
**-> (dash 30)
(hear 138 18 shoot the ball)
(see 139 ((flag r t) 38.1 -11) ((flag p r t) 22 -39) ((ball) 1.9 0) ((player usa 2) 12.8 27)
((player usa 3) 11.6 -27) ((line r) 25.5 -31))
**-> (say shooting now)
**-> (kick 53 51)
(hear 141 self shooting now)
(see 144 ((flag r t) 38.1 -11) ((flag p r t) 22 -39) ((ball) 8.1 42) ((player usa 2) 12.8 27)
((player usa 3) 11.6 -27) ((line r) 25.5 -31))
**-> (turn 42)
(see 149 ((goal r) 13.6 9) ((ball) 13.5 5 0) ((player usa 2) 12.8 -14) ((player brazil 1) 11 18)
((line r) 14 -73))
**-> (turn 5)
**-> (dash 81)
(hear 150 referee goal 1 1)
(hear 150 referee kick off r)
```



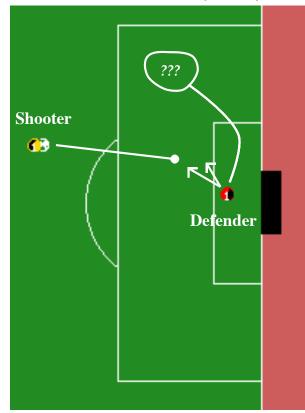
# simulated robotic soccer

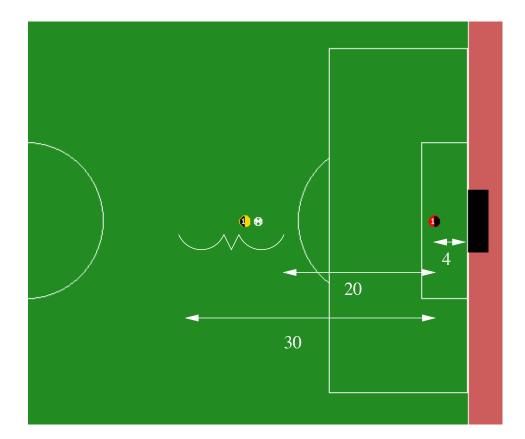
- An example of MAS;
- Enough complexity to be realistic;
- Easy accessibility to researchers worldwide;
- Embodiment of most MAS issues: reactivity, modeling, cooperation, competition, role playing, resource management, communication, convention, commitment/decommitment strategies
- Straightforward evaluation
- Good multiagent ML opportunities.

# Learning a lower-level skill

#### **Intercepting a moving ball:**

- Co-Learning for the shooter and the defender
- Using neural networks (NN)

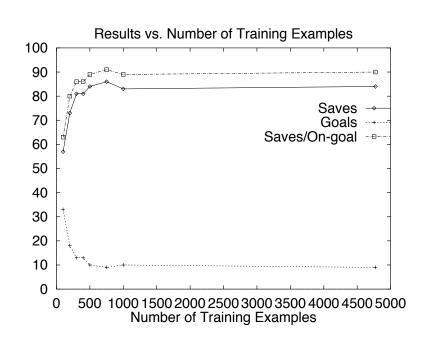




# Perfomance

A Layered Approach to Learning Client Behaviors in the RoboCup Soccer Server Peter Stone Manuela Veloso ?

Training			Saves
Examples	Saves(%)	Goals(%)	$\overline{\text{Goals+Saves}}(\%)$
100	57	33	63
200	73	18	80
300	81	13	86
400	81	13	86
500	84	10	89
750	86	9	91
1000	83	10	89
4773	84	9	90



# Learning a Higher-level Decision: pass, dribble, shoot

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# Learning a Higher-level Decision: passing

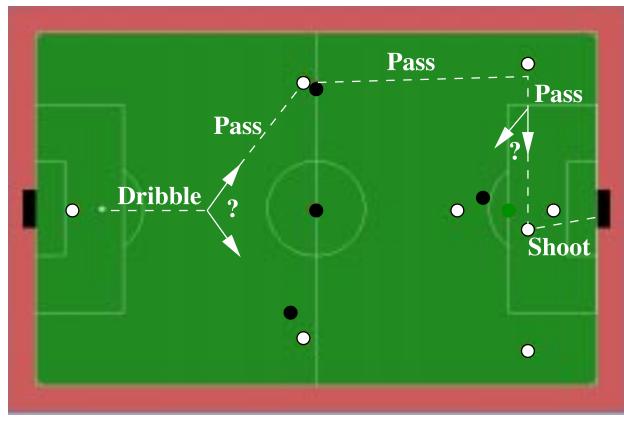
174 attributes were use to construct a Decision Tree:

- Distance and Angle to the receiver (2);
- ?Distance and Angle to other teammates (up to 9) sorted by angle from the receiver (18);
- Distance and Angle to opponents (up to 11) sorted by angle from the receiver (22);
- Counts of teammates, opponents, and players within given distances and angles of the receiver (45);
- Distance and Angle from receiver to teammates (up to 10) sorted by distance (20);
- ?Distance and Angle from receiver to opponents (up to 11) sorted by distance (22);
- Counts of teammates, opponents, and players within given distances and angles of the passer from the receiver's perspective (45);

		Success Confidence:			
Result	Overall	.8–.9	.7–.8	.6–.7	
(Number)	(5000)	(1050)	(3485)	(185)	
SUCCESS (%)	65	79	63	58	
FAILURE (%)	26	15	29	31	
MISS (%)	8	5	8	10	

# **Team-level Strategies**

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○ Teammate



## Next layers:

- More flexible and powerful approach would be to allow the dribbling player to learn:
  - when to continue dribbling,
  - when to pass, and
  - when to shoot.
- With these three possibilities as the action space and with appropriate predicates to discretize the state space, TD-lambda and other reinforcement learning methods will be applicable.
- By keeping track of whether an opponent or a teammate possesses the ball next, a player can propagate reinforcement values for each decision made while it possesses the ball.

# Next layer

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- Learning moving behavior to be a targeted receiver
- Learn to cooperate with the teammates, learn to thwart the opponents
- Last updates allow to have one more agent: the coach (trainer)

# **ROBOCUP:** summary



#### Layered Learning in Multiagent Systems

A Winning Approach to Robotic Soccer

Peter Stone

# The Dream

We proposed that the ultimate goal of the RoboCup Initiative to be stated as follows:

- By the middle of the 21st century, a team of fully autonomous humanoid robot soccer players shall win a soccer game, complying with the official rules of FIFA, against the winner of the most recent World Cup.
- Challenging project that cover many issues in AI and Data Science
- P. Stone. Layered Learning in Multiagent Systems : A Winning Approach to Robotic Soccer.
- Why soccer (football)?

# Semantic text processing

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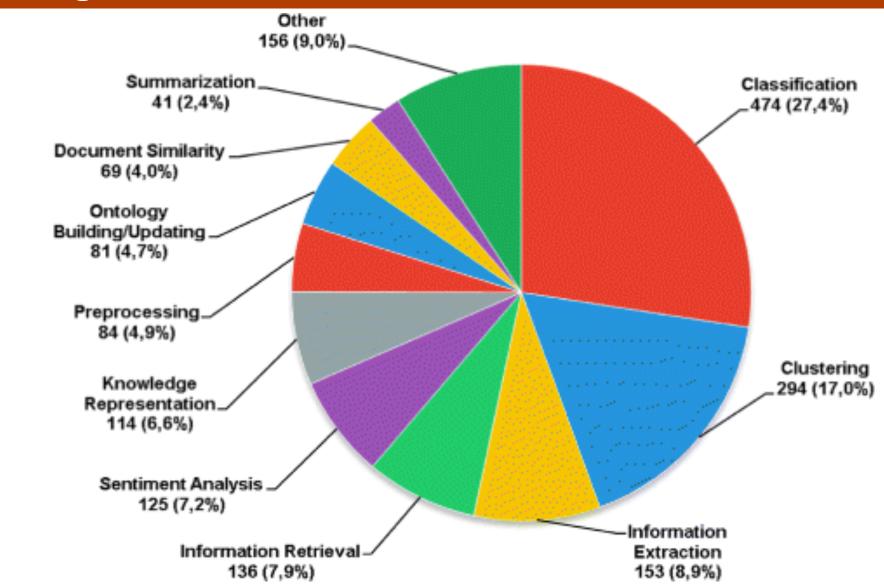
### What for?

- Extract relevant and useful information from large bodies of unstructured data
- Find an answer to a question without having to ask a human
- Discover the meaning of colloquial speech in online posts
- Uncover specific meanings of words used in foreign languages mixed with our own

#### Semantic text mining tasks:

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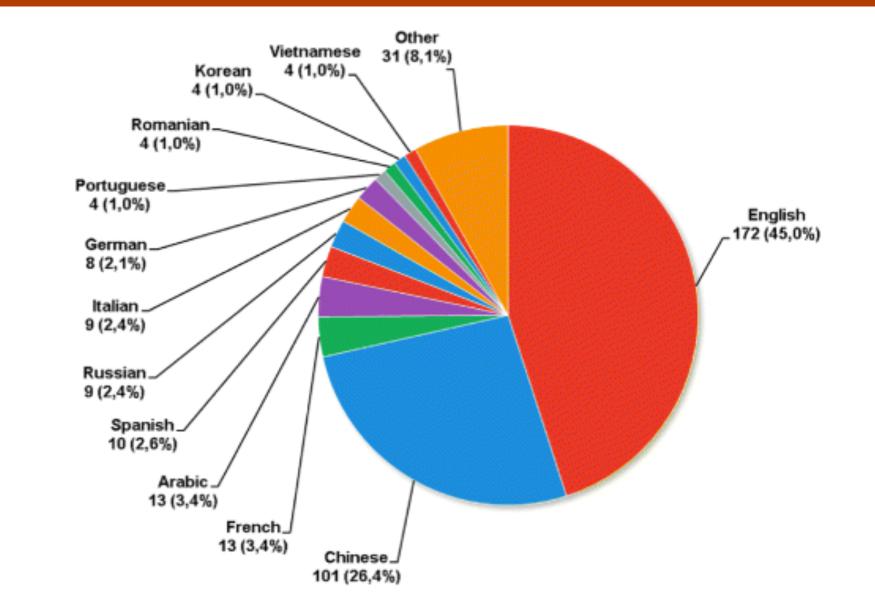
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# What are the natural languages being considered when working with text semantics?

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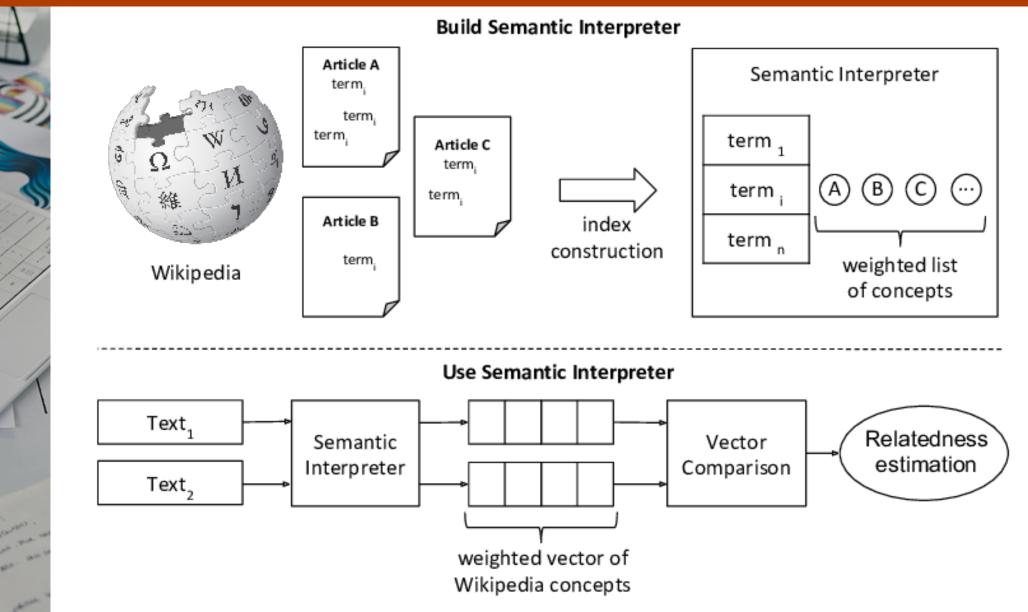
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#### Explicit Semantic Analysis (ESA)

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## Semantic interpreter

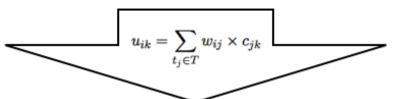
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		term <sub>0</sub>	term <sub>1</sub>		term <sub>M</sub>
doc	)	$W_{00}$	$W_{01}$		$w_{0M}$
doc	1	$W_{10}$			
				Wij	
doc	N	$W_{\rm N0}$			W <sub>NM</sub>

Representation of system data

	concept <sub>0</sub>	concept1	oncept <sub>1</sub>		
term <sub>0</sub>	$C_{00}$	$C_{01}$		С <sub>0К</sub>	
term <sub>1</sub>	$C_{10}$				
term <sub>M</sub>	$c_{\rm M0}$			$\mathcal{C}_{\mathrm{MK}}$	

#### Representation of knowledge base



	concept <sub>0</sub>	concept1		concept <sub>K</sub>	
doc <sub>0</sub>	$u_{00}$	$u_{01}$		$u_{0\mathrm{K}}$	
doc <sub>1</sub>	$u_{10}$				
			$u_{ik}$		
doc <sub>N</sub>	$u_{ m N0}$			<i>u</i> <sub>NK</sub>	

#### New representation of system data

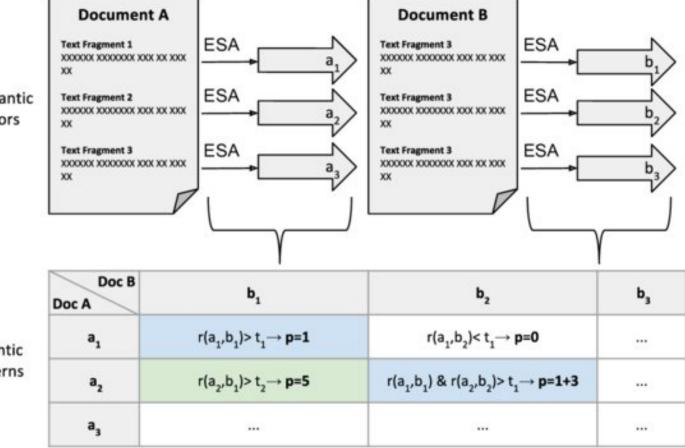
#### Example: Semantic similarity

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extracting semantic concept vectors

scoring semantic concept patterns

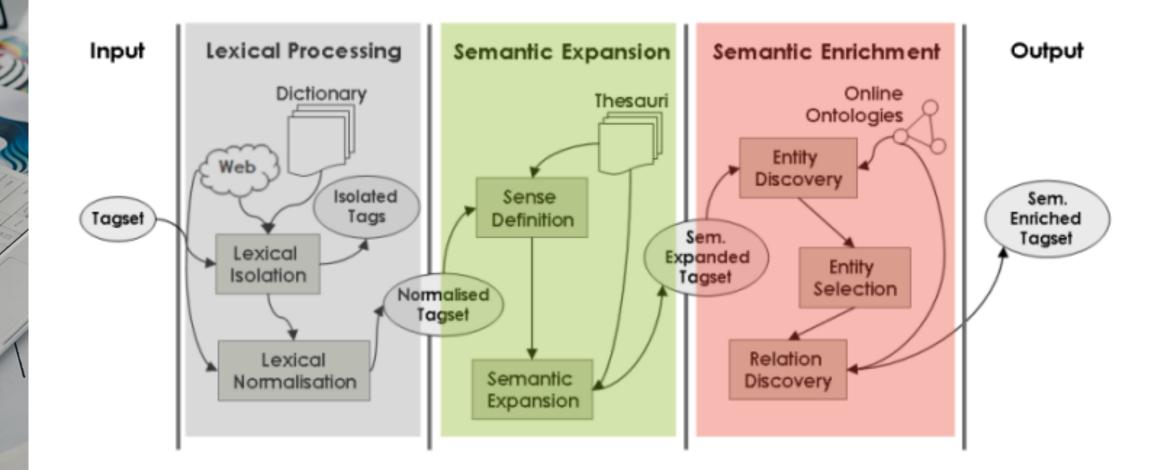


#### Semantic enrichment

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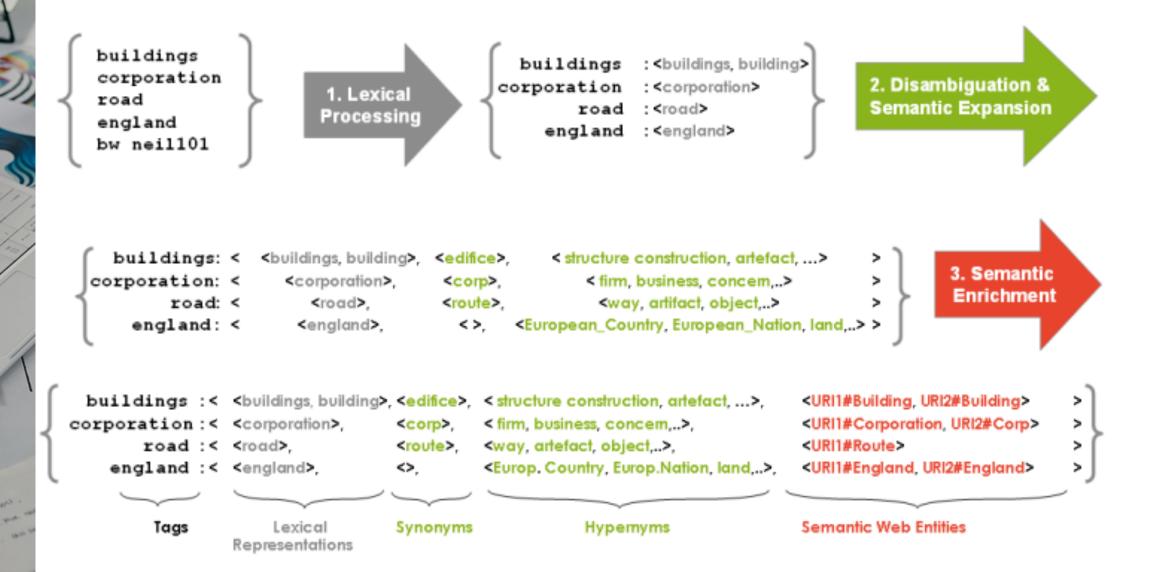
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#### Example

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## Improved ESA

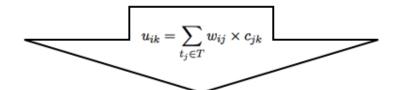
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	term <sub>0</sub>	term <sub>1</sub>		term <sub>M</sub>	
doc <sub>0</sub>	$W_{00}$	$W_{01}$		$W_{0M}$	
doc <sub>1</sub>	$W_{10}$				
			Wij		
doc <sub>N</sub>	$W_{\rm N0}$			WNM	

Representation of system data

	concept <sub>0</sub>	concept1		concept <sub>K</sub>	
term <sub>0</sub>	$C_{00}$	$C_{01}$		$\mathcal{C}_{0\mathrm{K}}$	
term <sub>1</sub>	$C_{10}$				
			$c_{jk}$		
term <sub>M</sub>	$c_{\rm M0}$			$c_{\rm MK}$	

Representation of knowledge base



	concept <sub>0</sub>	concept1		concept <sub>K</sub>
doc <sub>0</sub>	$u_{00}$	$u_{01}$		$u_{0\mathrm{K}}$
doc <sub>1</sub>	$u_{10}$			
			$u_{ik}$	
doc <sub>N</sub>	$u_{ m N0}$			<i>u</i> <sub>NK</sub>



New representation of system data

#### JRS'2012 Data mining competition

Large biomedical document repositories, such as MEDLINE, hire experts to index their resources with MeSH terms.

- MeSH contains over 26,000 main *headings*.
- Headings can be used in a context of 83 qualifiers (*subheadings*).
- Medical doctors use MeSH heading/subheading pairs to search for information.
- 670,943 articles were indexed (semi-)manually in 2007.



Experts need support in their work.

• Over 1 million articles are expected in 2015...

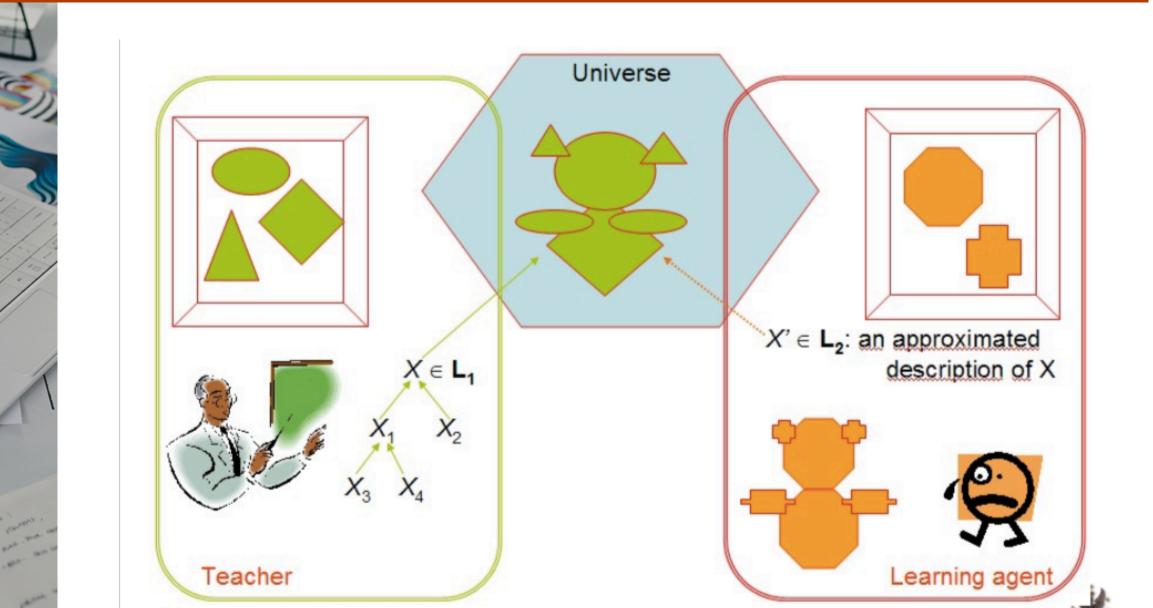
### Challenges

- Scalability: deeper semantic analysis vs time and space complexity
- Text representation model.
- Semantic analysis < text understanding
- Example: Named Entity Recognition (NER) problem:
  - One of the major problems in NER is ambiguous names: e.g. one protein name may refer to multiple gene products
  - Example: using sense-tagged corpora and unified medical language system (UMLS) to resolve ambiguous terms.
     Machine-learning techniques have been applied to sense-tagged corpora, in which senses (or concepts) of ambiguous terms have been most manually annotated
    - >>> quite an expansive manual work

#### Concept approximation

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#### Example nursery data set

- Creator: Vladislav Rajkovic et al. (13) experts)
- Donors: Marko Bohanec ۲ (marko.bohanec@ijs.si) Blaz Zupan (blaz.zupan@ijs.si)

- Date: June, 1997
- Number of Instances: 12960 ۲ (instances completely cover the attribute space)

prior

Number of Attributes: 8 ۲

#### Attributes

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NURSERY	not_recom, recommend, very_recom, priority, spec
. EMPLOY	Employment of parents and child's nursery
parents	usual, pretentious, great_pret
has_nurs	proper, less_proper, improper, critical, very_crit
. STRUCT_FINAN	Family structure and financial standings
STRUCTURE	Family structure
form	complete, completed, incomplete, foster
children	1, 2, 3, more
housing	convenient, less_conv, critical
finance	convenient, inconv
. SOC_HEALTH	Social and health picture of the family
social	non-prob, slightly_prob, problematic
health	recommended, priority, not recom

#### Layered learning

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#### Method:

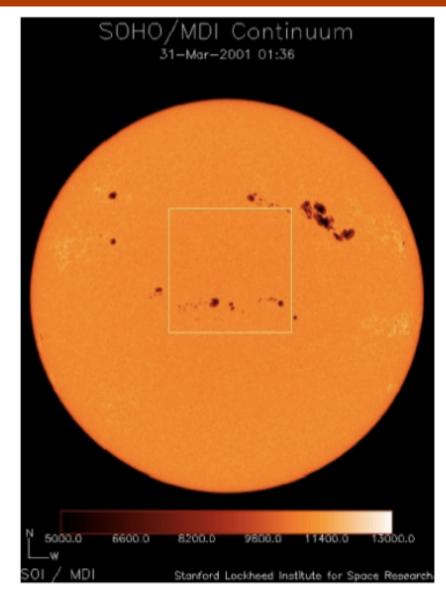
- Use clustering algorithm to approximate intermediate concepts;
- Use rule based algorithm (RSES system) to approximate the target concept;

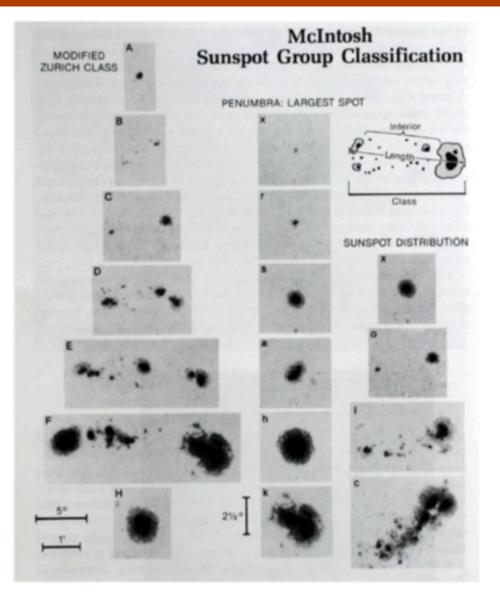
#### Results: (60% - training, 40% - testing )

`		• /
	original attributes only	using intermediate concepts
Accuracy	83.4	99.9%
Coverage	85.3%	100%
Nr of rules	634	42 (for the target concept)
		92 (for intermediate concepts)

## Sunspot recognition and classification

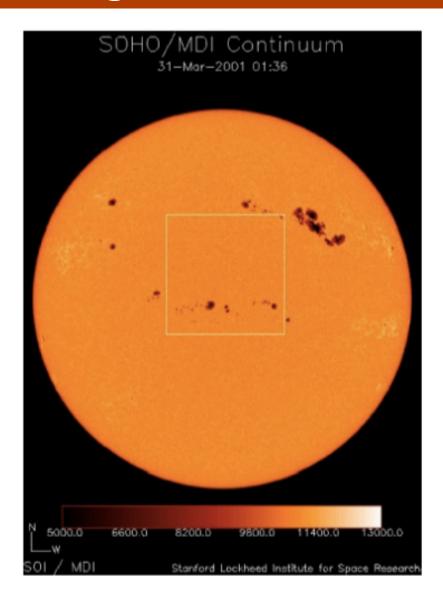


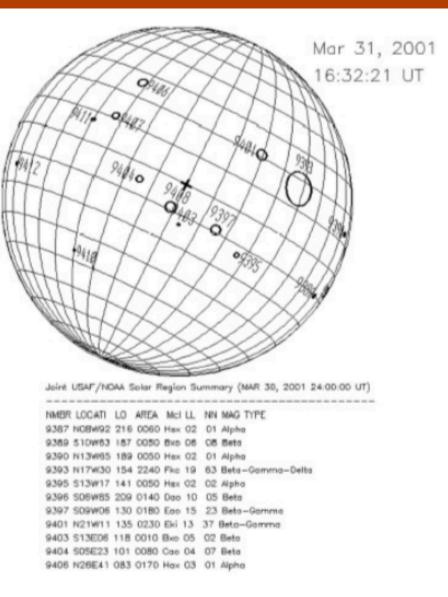




#### Sunspot recognition and classification







#### **Differential Calculus to Function Approximation**

- ill-defined data: limited number of objects and large number of attributes;
- prediction of a real decision variable based on nominal attributes;
- the need for the knowledge about the real mechanisms behind the data;

No.	Combination	B-1	1-4	4-6	6-E	PB	ΡE	Binding affinity
1	A2B2C2D2a2b2	1	1	1	1	1	1	4.52526247
2	A1B2C1D1a2b2	-1	1	-1	-1	1	1	4.818066119
3	A1B2C2D1a2b2	-1	1	1	-1	1	1	5.036009902
39	A1B1C1D1a1b1	-1	-1	-1	-1	-1	-1	8.963821581
40	A1B1C1D1a2b1	-1	-1	-1	-1	1	-1	8.998482244

#### **Discrete Differential Calculus**



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1. A (	decisi	on ta	ble	
S	$a_1$	dec		
$u_1$	1	-1		4.23
$u_2$	1	1		4.31
$u_n$	-1	1		8.92

2. Domain knowledge

#### First level

• Create comparing table

	$a_1$	$a_2$	 change
$u_1, u_2$	$1 \rightarrow 1$	$-1 \rightarrow 1$	 7
$u_1, u_3$			 $\searrow$

 Learn the preference relation, i.e., decision rules of form

$$a_2: -1 \rightarrow 1 \land a_6 = 1... \implies change = \searrow$$

#### Second level

- Ranking prediction;
- Decision value prediction;
- Experiment design.

#### Semantic evaluation of clustering algorithm.









Which partition is better?



#### External evaluation methods

Doc.	Soft Cluster			Expert Tag				
	$C_1$	$C_2$	$C_3$	Cosmonaut	astronaut	moon	car	truck
$d_1$	1			1		1	1	
$d_2$	1				1	1		
$d_3$	1	1		1				
$d_4$		1	1				1	1
$egin{array}{c} d_5 \ d_6 \end{array}$		1	1				1	
$d_6$			1					1

#### Rand index:

Pairs of documents		Same cluster?	
		Yes	No
Same	Yes	a	b
expert tag?	No	c	d

## MMI (Maximum Mutual Information):

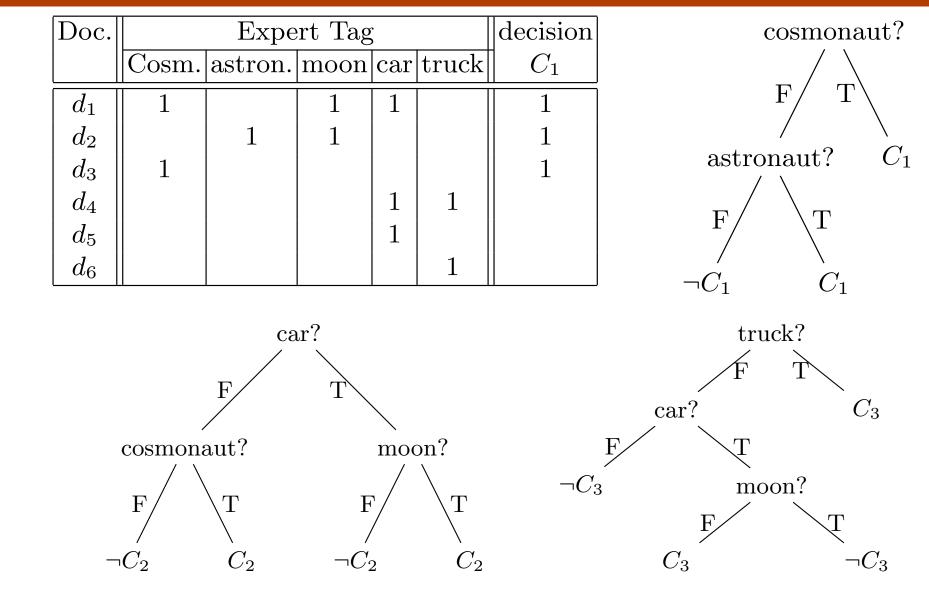
	$C_1$	$C_2$	$C_3$
Cosmonaut	0.139	0.083	0
astronaut	0.083	0	0
moon	0.139	0	0
car	0.056	0.125	0.125
truck	0	0.042	0.208

$$MMI(X,Y) = \sum_{x} \sum_{y} p(x,y) \log\left(\frac{p(x,y)}{p(x)p(y)}\right)$$

Rand Index = 
$$\frac{a+d}{a+b+c+d}$$
.

#### Semantic Explorative Evaluation

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## Learning Ontology

### Ontology learning

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- Ontology Learning from Text:
- Linked Data Mining
- Concept Learning in Description Logics and OWL
- Crowdsourcing

#### Challenges in ontology learning

- *Heterogeneity:* neither the integration of methods nor the homogenization of data has attracted high attention of ML community
- **Uncertainty:** Low-quality or unstructured data can lead to results that are less likely to be correct.
- Reasoning: ontology learning approaches are not capable of generating consistent (and coherent) ontologies
- Scalability: Extracting knowledge from the growing amounts of data on the web – un-structured, textual data on the one hand and structured data such as databases, linked data or ontologies on the other hand – requires scalable and efficient approaches
- **Quality:** Formal correctness, completeness and consistency are only a few of many possible criteria for judging the quality of an ontology
- *Interactivity:* The lesser the extent to which humans are involved in a semiautomatic ontology generation process, the lower the quality we can expect.

#### CONCLUSIONS

- No free lunch theorem =>
  - a need of knowledge modeling and involving in the learning process
- Layered learning = decomposition + synthesis of results
- Lack of a "back propagation" mechanism
- ML techniques are efficient in Knowledge Acquisition