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# Advanced Natural Language Processing and Information Retrieval

## PART I: Essential Notions of Information Retrieval and Machine Learning

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#### Outline

- Motivation
  - Question Answering vs. Search Engines
- Information Retrieval Techniques
  - Search Engines
  - Vector Space Model
  - Feature Vectors and Feature Selection
  - Text Categorization
  - Measures
- Machine Learning Methods
  - Classification
  - Ranking
  - Regression (logistic)



#### Outline

- Natural Language tools and techniques
  - Lemmatization
  - POS tagging
  - NER + gazetteer look up
  - Dependency and Constituency trees
  - Predicate Argument Structure
- Question Answering Pipeline
  - Similarity for supporting answers
  - QA tasks (open, restricted, factoid, non-factoid)



#### Motivations

- Approach to automatic Question Answering Systems
  - 1. Extract query keywords from the question
  - 2. Retrieve candidate passages containing such keywords (or synonyms)
  - 3. Select the most promising passage by means of query and answer similarity
- For example
  - Who is the President of the United States?
  - (Yes) The president of the United States is Barack Obama
  - (no) Glenn F. Tilton is President of the United Airlines



AlchemyAPI – Named Enti	ty Extra FreeLing 3.0 - Demonstration 🛛 who is the president of the unite when hit by electrons, a phospho
+Alessandro Sea	rch Images Maps YouTube Gmail Documents Calendar Translate More -
Google	Who is the President of the United States? Q Alessa
Search	About 3,220,000,000 results (1.09 seconds)
Everything	Best guess for United States of America President is Barack
Images	Obama
Maps	Mentioned on at least 3 websites including wikipedia.org, whitehouse.gov and youtube.com - Show sources - Feedback
Videos	
News	President of the United States - Wikipedia, the free encyclo en.wikipedia.org/wiki/President_of_the_United_States
Shopping	Incumbent Barack Obama since January 20, 2009. Style, Mr.
More	President (informal) The Honorable (formal) His Excellency (diplomatic, outside the U.S.)
Trento	Origin - Powers and duties - Selection process - Compensation
Change location	List of Presidents of the United States - Wikipedia, the free en.wikipedia.org/wiki/List_of_Presidents_of_the_United_States
Show search tools	John F. Kennedy was the first <b>president</b> of Roman Catholic faith, and the current <b>president</b> , <b>Barack Obama</b> , is the first <b>president</b> of African- American descent;

#### The Presidents | The White House

. . . . . . . . . . . .

#### **Motivations**

- TREC has taught that this model is to weak
- Consider a more complex task, i.e. a Jeopardy cue
- When hit by electrons, a phosphor gives off electromagnetic energy in this form
  - Solutions: *photons/light*
- What are the most similar fragments retrieved by a search engine?





When hit by electrons, a phosphor gives off electromagnetic energy



About 194,000 results (0.22 seconds)

Advan

#### Cathode-Ray Tube - body, used, chemical, characteristics, form ... 2 2

Sep 6, 2010 ... In order to **form** the **electron** beam into the correct shape, ... The actual conversion of electrical **energy** to light **energy** takes place on the ... For example, the **phosphor** known as yttrium oxide **gives off** a red glow ... complete explanation of electrostatic and **electromagnetic** focusing in the crt ...

www.scienceclarified.com > Ca-Ch - Cached - Similar

#### Beta particle - Wikipedia, the free encyclopedia 😭 🔍

Beta particles are high-energy, high-speed electrons or positrons emitted by certain ... The beta particles emitted are a form of ionizing radiation also known as beta rays. ... by electromagnetic interactions and may give off bremsstrahlung x-rays. ... The well-known 'betalight' contains tritium and a phosphor. ...

en.wikipedia.org/wiki/Beta\_particle - Cached - Similar

#### luminescence: Definition from Answers.com

Included on the **electromagnetic** spectrum are radio waves and microwaves; ... Though the Sun sends its **energy** to Earth in the **form** of light and heat from the .... Thanks to the **phosphor**, a fluorescent lamp **gives off** much more light than an ... The tube itself is coated

#### Motivations (2)

- This shows that:
  - Lexical similarity is not enough
  - Structure is required
- What kind of structures do we need?
- How to carry out structural similarity?



#### **Information Retrieval Techniques**

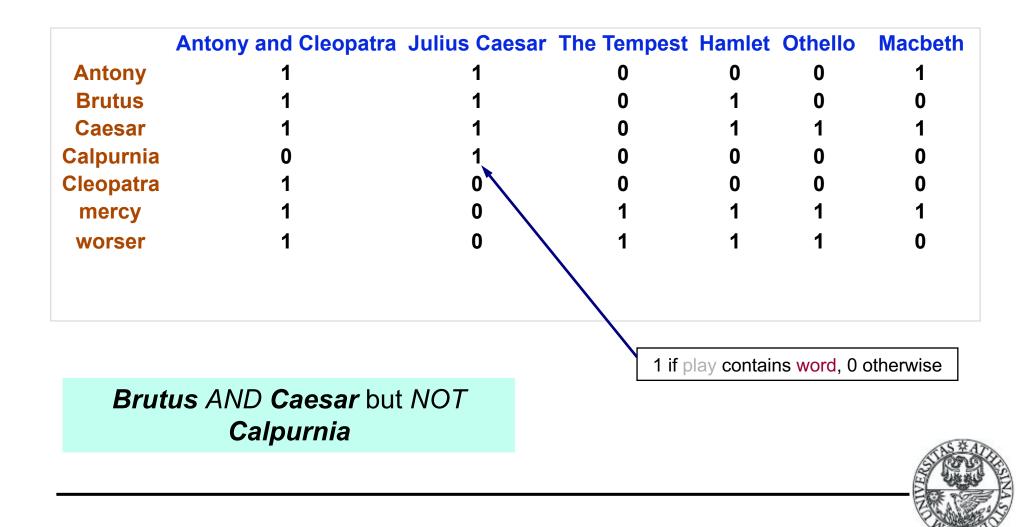


# **Indexing Unstructured Text**

- Which plays of Shakespeare contain the words Brutus AND Caesar but NOT Calpurnia?
- One could grep all of Shakespeare's plays for Brutus and Caesar, then strip out lines containing Calpurnia?
  - Slow (for large corpora)
  - <u>NOT</u> Calpurnia is non-trivial
  - Other operations (e.g., find the word *Romans* near *countrymen*) not feasible
  - Ranked retrieval (best documents to return)



#### **Term-document incidence**



- So we have a 0/1 vector for each term.
- To answer query: take the vectors for *Brutus, Caesar* and *Calpurnia* (complemented) ⇒
   bitwise *AND*.
- 110100 AND 110111 AND 101111 = 100100.

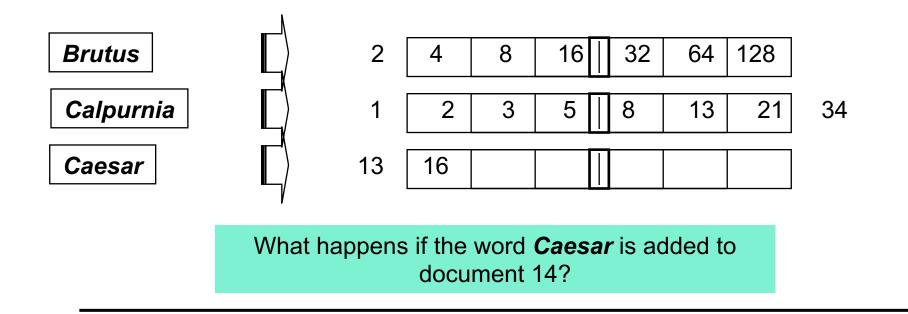


### **Term-document incidence**

ot Calpurnia	1	0	0	1	0	0
Antor	ny and Cleopatra	Julius Caesar	The Tempest	Hamlet	Othello	Macbeth
Antony	1	1	0	0	0	1
Brutus	1	1	0	1	0	0
Caesar	1	1	0	1	1	1
Calpurnia	0	1	0	0	0	0
Cleopatra	1	0	0	0	0	0
mercy	1	0	1	1	1	1
worser	1	0	1	1	1	0
			$\mathbf{h}$			
			<b>1</b> if p	lay contair	ns word, 0	otherwise
Brutus Al	VD <b>Caesar</b> bu	t <i>NOT</i>				
	Calpurnia					SUNS

For each term T, we must store a list of all documents that contain T.

Do we use an array or a list for this?

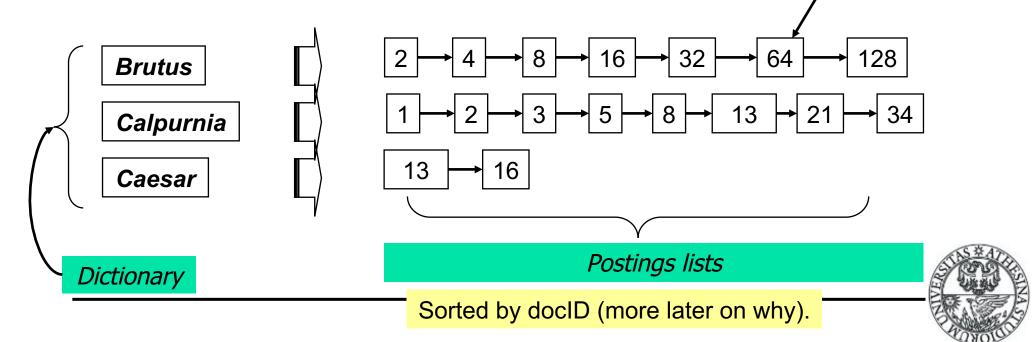




## Inverted index

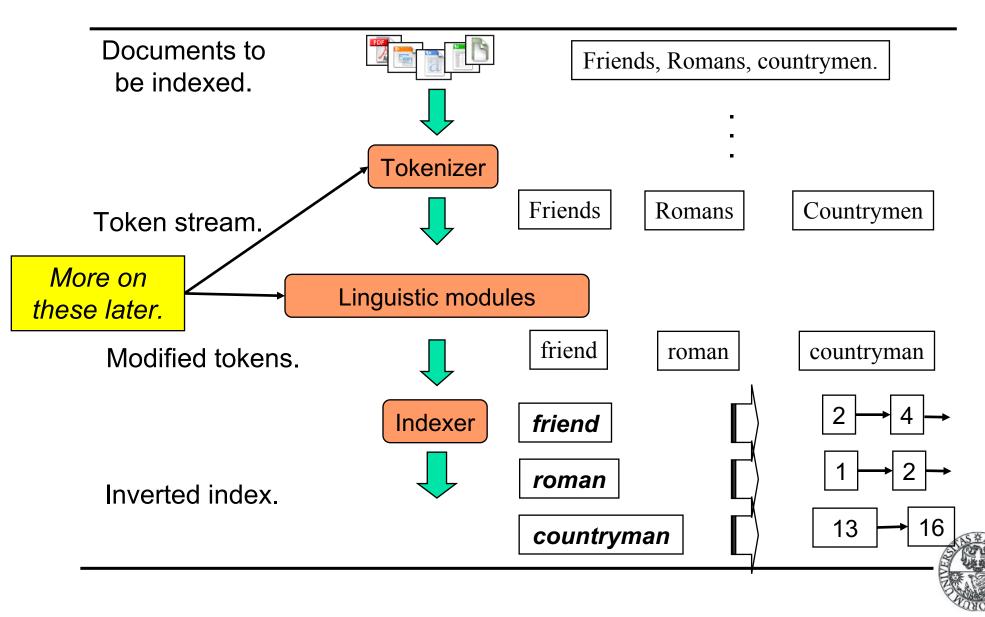
Linked lists generally preferred to arrays

- Dynamic space allocation
- Insertion of terms into documents easy
- Space overhead of pointers

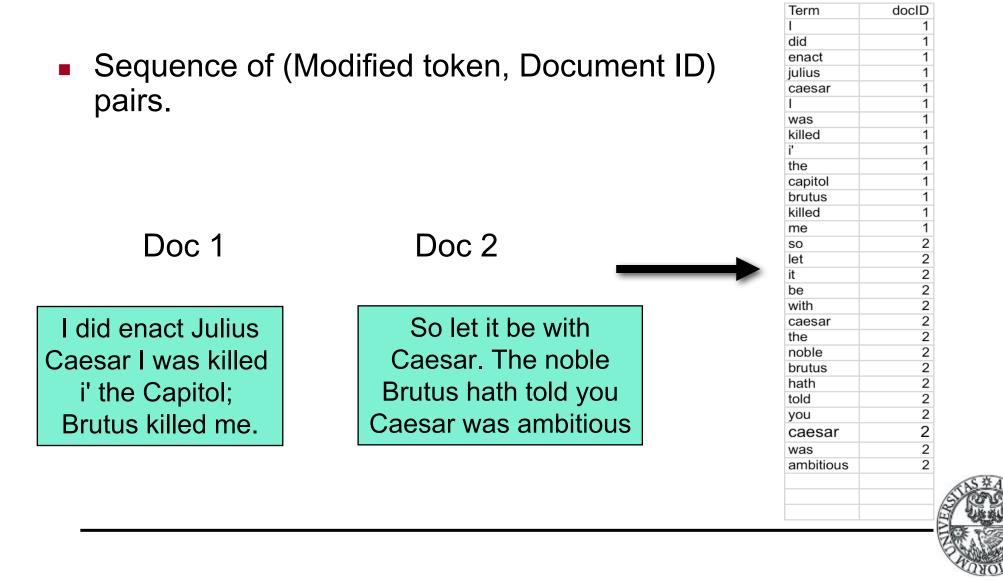


Posting

#### **Inverted index construction**



## **Indexer steps**



#### Sort by terms.

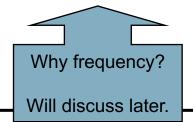


_			
Term	docID	Term	docID
1	1	ambitious	2
did	1	be	2
enact	1	brutus	2
julius	1	brutus	2
caesar	1	capitol	1
1	1	caesar	1
was	1	caesar	2
killed	1	caesar	2
i'	1	did	1
the	1	enact	1
capitol	1	hath	1
brutus	1	1	1
killed	1		1
me	1	i	1
SO	2	it	2
let	2	julius	1
it	2	killed	1
be	2	killed	1
with	2	let	2
caesar	2	me	2
the	2	noble	2
noble	2	SO	2 2 1
brutus	2	the	1
hath	2	the	2 2 2 1
told	2	told	2
you	2	you	2
caesar	2	was	1
was	2	was	2
ambitious	2	with	2



#### **Indexer steps: Dictionary & Postings**

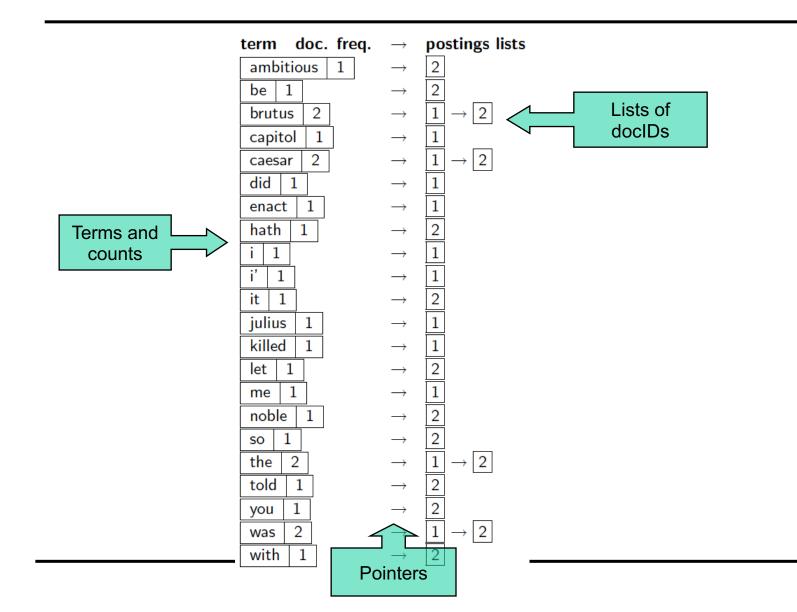
- Multiple term entries in a single document are merged.
- Split into Dictionary and Postings
- Doc. frequency information is added.



Town	de - ID	term doc. freq.	$\rightarrow$	postings lists
Term	docID	ambitious 1	$\rightarrow$	2
ambitious	2			
be brutus	2	be 1	$\rightarrow$	2
brutus	2	brutus 2	$\rightarrow$	$1 \rightarrow 2$
capitol	1	capitol 1	$\rightarrow$	1
caesar	1		-	
caesar	2	caesar 2	$\rightarrow$	$ 1  \rightarrow  2 $
caesar	2	did 1	$\rightarrow$	1
did	1			
enact	1	enact 1	$\rightarrow$	1
hath	1	hath 1	$\rightarrow$	2
1	1			
1	1	i 1	$\rightarrow$	1
i'	1	i' 1	$\rightarrow$	1
it	2	it 1		2
julius	1		_	
killed	1	julius 1	$\rightarrow$	1
killed	1	killed 1	$\rightarrow$	1
let	2			
me	1	let   1	$\rightarrow$	2
noble	2	me 1	$\rightarrow$	1
SO	2			
the	1	noble 1	$\rightarrow$	2
the	2	so 1	$\rightarrow$	2
told	2			
you	2	the 2	$\rightarrow$	$1 \rightarrow 2$
was	1	told 1	$\rightarrow$	2
was	2			
with	2	<u> </u>	$\rightarrow$	2
		was 2	$\rightarrow$	$ 1  \rightarrow  2 $
		with 1	$\rightarrow$	2



#### Where do we pay in storage?





# **Query processing: AND**

Consider processing the query:

#### Brutus AND Caesar

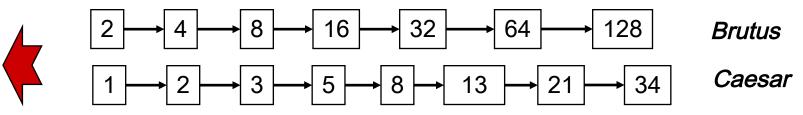
#### Locate *Brutus* in the Dictionary;

Retrieve its postings.

Locate Caesar in the Dictionary;

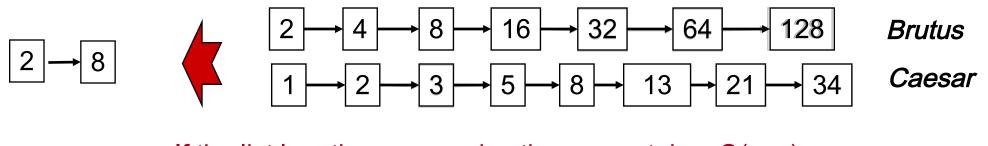
Retrieve its postings.

"Merge" the two postings:





Walk through the two postings simultaneously, in time linear in the total number of postings entries



If the list lengths are x and y, the merge takes O(x+y)

operations.

Crucial: postings sorted by docID.



## **Boolean queries: Exact match**

- The Boolean Retrieval model is being able to ask a query that is a Boolean expression:
  - Boolean Queries are queries using AND, OR and NOT to join query terms
    - Views each document as a <u>set</u> of words
    - Is precise: document matches condition or not.
- Primary commercial retrieval tool for 3 decades.
- Professional searchers (e.g., lawyers) still like Boolean queries:
  - You know exactly what you' re getting.



#### **Evidence accumulation**

- 1 vs. 0 occurrence of a search term
  - 2 vs. 1 occurrence
  - 3 vs. 2 occurrences, etc.
  - Usually more seems better
- Need term frequency information in docs



#### **Ranking search results**

- Boolean queries give inclusion or exclusion of docs.
- Often we want to rank/group results
  - Need to measure proximity from query to each doc.
  - Need to decide whether docs presented to user are singletons, or a group of docs covering various aspects of the query.



## IR vs. databases: Structured vs unstructured data

Structured data tends to refer to information in "tables"

Employee	Manager	Salary
Smith	Jones	50000
Chang	Smith	60000
lvy	Smith	50000

Typically allows numerical range and exact match (for text) queries, e.g., Salary < 60000 AND Manager = Smith.



#### **Unstructured data**

- Typically refers to free-form text
- Allows
  - Keyword queries including operators
  - More sophisticated "concept" queries, e.g.,
    - find all web pages dealing with drug abuse
- Classic model for searching text documents



- In fact almost no data is "unstructured"
- E.g., this slide has distinctly identified zones such as the *Title* and *Bullets*
- Facilitates "semi-structured" search such as
  - Title contains <u>data</u> AND Bullets contain <u>search</u>

... to say nothing of linguistic structure



# From Binary term-document incidence matrix

	Antony and Cleopatra	Julius Caesar	The Tempest	Hamlet	Othello	Macbeth
Antony	1	1	0	0	0	1
Brutus	1	1	0	1	0	0
Caesar	1	1	0	1	1	1
Calpurnia	0	1	0	0	0	0
Cleopatra	1	0	0	0	0	0
mercy	1	0	1	1	1	1
worser	1	0	1	1	1	0

#### Each document is represented by a binary vector $\in \{0,1\}|V|$



#### **To term-document count matrices**

- Consider the number of occurrences of a term in a document:
  - Each document is a count vector in N<sup>v</sup>: a column below

	Antony and Cleopatra	Julius Caesar	The Tempest	Hamlet	Othello	Macbeth
Antony	157	73	0	0	0	0
Brutus	4	157	0	1	0	0
Caesar	232	227	0	2	1	1
Calpurnia	0	10	0	0	0	0
Cleopatra	57	0	0	0	0	0
mercy	2	0	3	5	5	1
worser	2	0	1	1	1	0



#### Bag of words model

- Vector representation doesn't consider the ordering of words in a document
- John is quicker than Mary and Mary is quicker than John have the same vectors
- This is called the <u>bag of words</u> model.
- In a sense, this is a step back: The positional index was able to distinguish these two documents.



#### **Term frequency tf**

- The term frequency tf<sub>t,d</sub> of term t in document d is defined as the number of times that t occurs in d.
- We want to use tf when computing query-document match scores. But how?
- Raw term frequency is not what we want:
  - A document with 10 occurrences of the term is more relevant than a document with 1 occurrence of the term.
  - But not 10 times more relevant.
- Relevance does not increase proportionally with term frequency.
  NB: frequency = count in IR

#### **Log-frequency weighting**

The log frequency weight of term t in d is

$$w_{t,d} = \begin{cases} 1 + \log_{10} tf_{t,d}, & \text{if } tf_{t,d} > 0\\ 0, & \text{otherwise} \end{cases}$$

- $0 \rightarrow 0, 1 \rightarrow 1, 2 \rightarrow 1.3, 10 \rightarrow 2, 1000 \rightarrow 4, \text{etc.}$
- Score for a document-query pair: sum over terms t in both q and d:

• score = 
$$\sum_{t \in q \cap d} (1 + \log tf_{t,d})$$

The score is 0 if none of the query terms is present in the document.



#### **Document frequency**

- Rare terms are more informative than frequent terms
  - Recall stop words
- Consider a term in the query that is rare in the collection (e.g., *arachnocentric*)
- A document containing this term is very likely to be relevant to the query *arachnocentric*
- → We want a high weight for rare terms like arachnocentric.



#### idf weight

- df<sub>t</sub> is the <u>document</u> frequency of t: the number of documents that contain t
  - df<sub>t</sub> is an inverse measure of the informativeness of t
  - $df_t \leq N$
- We define the idf (inverse document frequency) of t by  $idf_t = log_{10} (N/df_t)$ 
  - We use log (N/df<sub>t</sub>) instead of N/df<sub>t</sub> to "dampen" the effect of idf.

Will turn out the base of the log is immaterial.



#### tf-idf weighting

The tf-idf weight of a term is the product of its tf weight and its idf weight.

$$\mathbf{w}_{t,d} = \log(1 + \mathrm{tf}_{t,d}) \times \log_{10}(N/\mathrm{df}_t)$$

- Best known weighting scheme in information retrieval
  - Note: the "-" in tf-idf is a hyphen, not a minus sign!
  - Alternative names: tf.idf, tf x idf
- Increases with the number of occurrences within a document
- Increases with the rarity of the term in the collection



Score(q,d) = 
$$\sum_{t \in q \cap d} \text{tf} \times \text{idf}_{t,d}$$

- There are many variants
  - How "tf" is computed (with/without logs)
  - Whether the terms in the query are also weighted



#### Binary $\rightarrow$ count $\rightarrow$ weight matrix

	Antony and Cleopatra	Julius Caesar	The Tempest	Hamlet	Othello	Macbeth
Antony	5.25	3.18	0	0	0	0.35
Brutus	1.21	6.1	0	1	0	0
Caesar	8.59	2.54	0	1.51	0.25	0
Calpurnia	0	1.54	0	0	0	0
Cleopatra	2.85	0	0	0	0	0
mercy	1.51	0	1.9	0.12	5.25	0.88
worser	1.37	0	0.11	4.15	0.25	1.95

Each document is now represented by a real-valued vector of tf-idf weights  $\in R|V|$ 



#### **Documents as vectors**

- So we have a |V|-dimensional vector space
- Terms are axes of the space
- Documents are points or vectors in this space
- Very high-dimensional: tens of millions of dimensions when you apply this to a web search engine
- These are very sparse vectors most entries are zero.



- Key idea 1: Do the same for queries: represent them as vectors in the space
- Key idea 2: Rank documents according to their proximity to the query in this space
  - proximity = similarity of vectors
  - proximity ≈ inverse of distance
  - rank more relevant documents higher than less relevant documents



#### \* Sec. 6.3

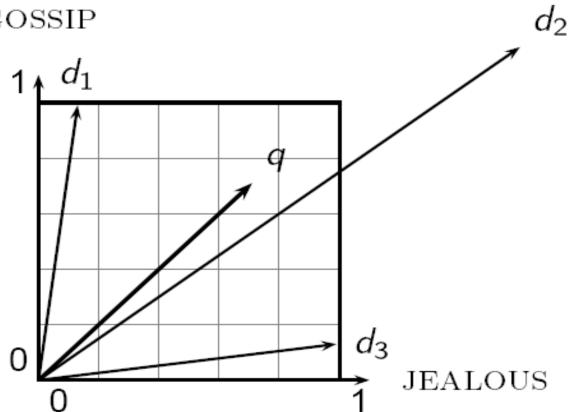
#### Formalizing vector space proximity

- First cut: distance between two points
  - ( = distance between the end points of the two vectors)
- Euclidean distance?
- Euclidean distance is a bad idea . . .
- ... because Euclidean distance is large for vectors of different lengths.



## Why distance is a bad idea

The Euclidean distance GOSSIP between  $\vec{q}$  $d_1$ and  $\vec{d_2}$  is large even though the distribution of terms in the query  $\vec{q}$  and the distribution of terms in the document  $\vec{d}_{2}$  are very similar.





#### Use angle instead of distance

- Thought experiment: take a document d and append it to itself. Call this document d'.
- "Semantically" d and d' have the same content
- The Euclidean distance between the two documents can be quite large
- The angle between the two documents is 0, corresponding to maximal similarity.
- Key idea: Rank documents according to angle with query.



#### From angles to cosines

The following two notions are equivalent.

- Rank documents in <u>decreasing</u> order of the angle between query and document
- Rank documents in <u>increasing</u> order of cosine (query,document)
- Cosine is a monotonically decreasing function for the interval [0°, 180°]



#### Length normalization

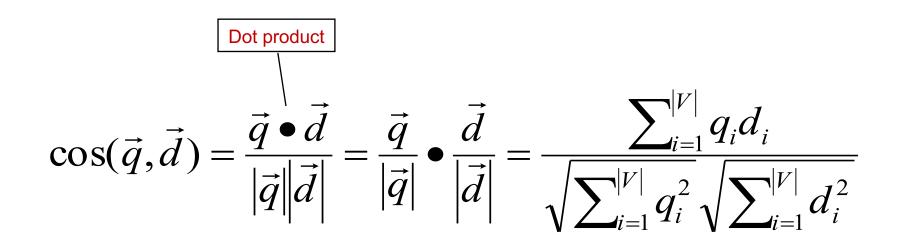
• A vector can be (length-) normalized by dividing each of its components by its length – for this we use the L<sub>2</sub> norm:  $\|\vec{x}\| = \sqrt{\sum x^2}$ 

$$\left\|\vec{x}\right\|_2 = \sqrt{\sum_i x_i^2}$$

- Dividing a vector by its L<sub>2</sub> norm makes it a unit (length) vector (on surface of unit hypersphere)
- Effect on the two documents d and d' (d appended to itself) from earlier slide: they have identical vectors after length-normalization.
  - Long and short documents now have comparable weights



#### cosine(query,document)



*qi* is the tf-idf weight of term *i* in the query *di* is the tf-idf weight of term *i* in the document

 $\cos(\vec{q}, \vec{d})$  is the cosine similarity of  $\vec{q}$  and  $\vec{d}$  ... or, equivalently, the cosine of the angle between  $\vec{q}$  and  $\vec{d}$ .



#### **Cosine for length-normalized vectors**

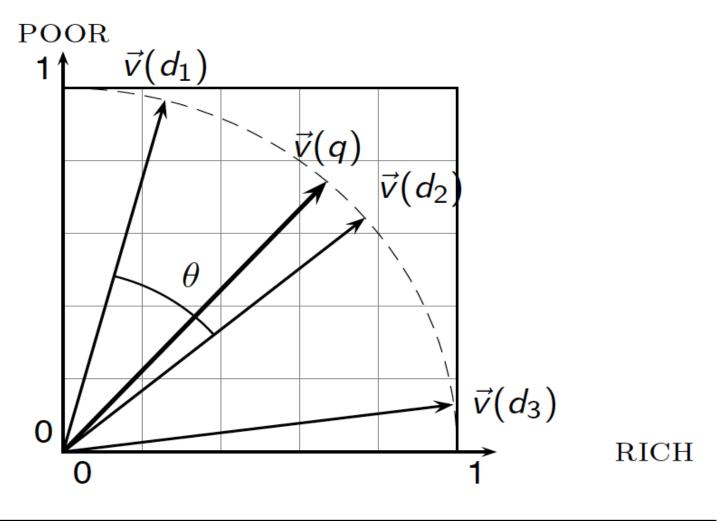
For length-normalized vectors, cosine similarity is simply the dot product (or scalar product):

$$\cos(\vec{q},\vec{d}) = \vec{q} \bullet \vec{d} = \sum_{i=1}^{|V|} q_i d_i$$

for q, d length-normalized.



#### **Cosine similarity illustrated**





#### **Performance Evaluation**



#### **Measures for a search engine**

- We can quantify speed/size
- Quality of the retrieved documents
- Relevance measurement requires 3 elements:
  - 1. A benchmark document collection
  - 2. A benchmark suite of queries
  - 3. A usually binary assessment of either <u>Relevant</u> or <u>Non</u> <u>relevant</u> for each query and each document
    - Some work on more-than-binary, but not the standard



#### **Evaluating an IR system**

- Note: the **information need** is translated into a **query**
- Relevance is assessed relative to the information need not the query
- E.g., <u>Information need</u>: I'm looking for information on whether drinking red wine is more effective at reducing your risk of heart attacks than white wine.
- Query: wine red white heart attack effective
- Evaluate whether the doc addresses the information need, not whether it has these words



#### Standard relevance benchmarks

- TREC National Institute of Standards and Technology (NIST) has run a large IR test bed for many years
- Reuters and other benchmark doc collections used
- "Retrieval tasks" specified
  - sometimes as queries
- Human experts mark, for each query and for each doc,
   <u>Relevant</u> or <u>Nonrelevant</u>
  - or at least for subset of docs that some system returned for that query



### Unranked retrieval evaluation: Precision and Recall

- Precision: fraction of retrieved docs that are relevant
   = P(relevant|retrieved)
- **Recall**: fraction of relevant docs that are retrieved
  - = P(retrieved | relevant)

	Relevant	Nonrelevant
Retrieved	tp	fp
Not Retrieved	fn	tn

- Precision P = tp/(tp + fp)
- Recall R = tp/(tp + fn)



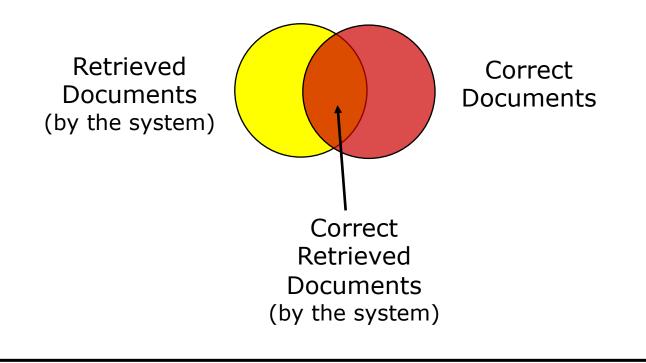
# Should we instead use the accuracy measure for evaluation?

- Given a query, an engine classifies each doc as "Relevant" or "Nonrelevant"
- The accuracy of an engine: the fraction of these classifications that are correct
  - (tp + tn) / (tp + fp + fn + tn)
- Accuracy is a evaluation measure in often used in machine learning classification work
- Why is this not a very useful evaluation measure in IR?



### **Performance Measurements**

- Given a set of document T
- Precision = # Correct Retrieved Document / # Retrieved Documents
- Recall = # Correct Retrieved Document/ # Correct Documents





#### Why not just use accuracy?

 How to build a 99.9999% accurate search engine on a low budget....



People doing information retrieval want to find something and have a certain tolerance for junk.



#### **Precision/Recall trade-off**

- You can get high recall (but low precision) by retrieving all docs for all queries!
- Recall is a non-decreasing function of the number of docs retrieved

- In a good system, precision decreases as either the number of docs retrieved or recall increases
  - This is not a theorem, but a result with strong empirical confirmation



#### A combined measure: F

Combined measure that assesses precision/recall tradeoff is F measure (weighted harmonic mean):

$$F = \frac{1}{\alpha \frac{1}{P} + (1 - \alpha) \frac{1}{R}} = \frac{(\beta^2 + 1)PR}{\beta^2 P + R}$$

People usually use balanced F<sub>1</sub> measure

• i.e., with 
$$\beta = 1$$
 or  $\alpha = \frac{1}{2}$ 

- Harmonic mean is a conservative average
  - See CJ van Rijsbergen, Information Retrieval

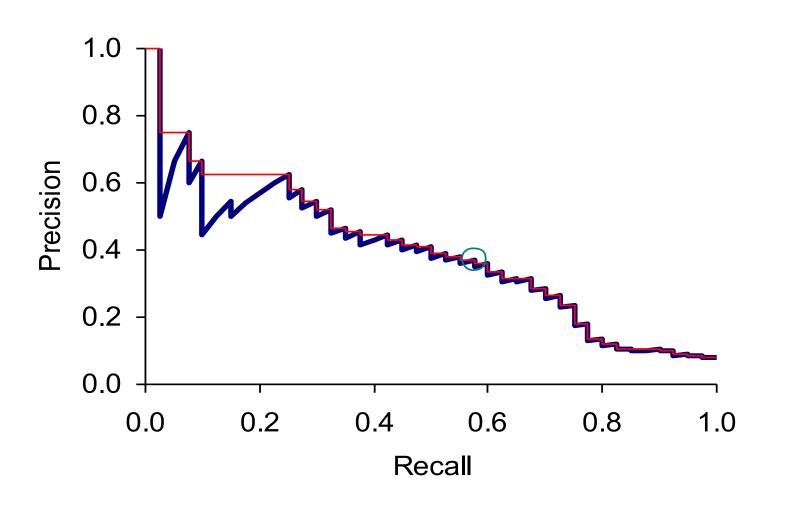


#### **Evaluating ranked results**

#### Evaluation of ranked results:

- The system can return any number of results
- By taking various numbers of the top returned documents (levels of recall), the evaluator can produce a *precisionrecall curve*





Sec. 8.4

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#### **Averaging over queries**

- A precision-recall graph for one query isn't a very sensible thing to look at
- You need to average performance over a whole bunch of queries.
- But there's a technical issue:
  - Precision-recall calculations place some points on the graph
  - How do you determine a value (interpolate) between the points?



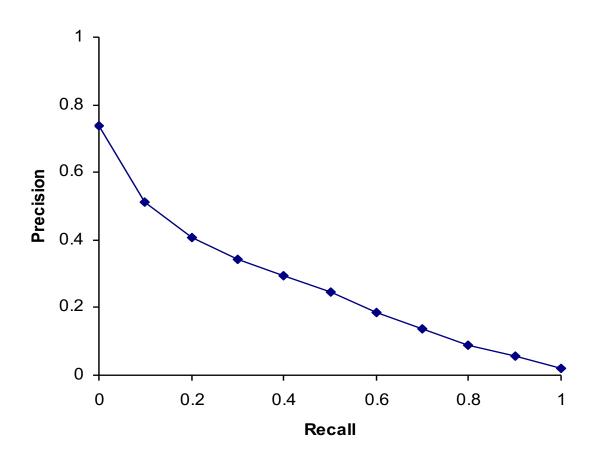
#### **Evaluation**

- Graphs are good, but people want summary measures!
  - Precision at fixed retrieval level
    - Precision-at-k: Precision of top k results
    - Perhaps appropriate for most of web search: all people want are good matches on the first one or two results pages
    - But: averages badly and has an arbitrary parameter of k
  - 11-point interpolated average precision
    - The standard measure in the early TREC competitions: you take the precision at 11 levels of recall varying from 0 to 1 by tenths of the documents, using interpolation (the value for 0 is always interpolated!), and average them
    - Evaluates performance at all recall levels



#### Typical (good) 11 point precisions

SabIR/Cornell 8A1 11pt precision from TREC 8 (1999)





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#### Yet more evaluation measures...

- Mean average precision (MAP)
  - Average of the precision value obtained for the top k documents, each time a relevant doc is retrieved
  - Avoids interpolation, use of fixed recall levels
  - MAP for query collection is arithmetic ave.
    - Macro-averaging: each query counts equally
- R-precision
  - If we have a known (though perhaps incomplete) set of relevant documents of size *Rel*, then calculate precision of the top *Rel* docs returned
  - Perfect system could score 1.0.



#### TREC

- TREC Ad Hoc task from first 8 TRECs is standard IR task
  - 50 detailed information needs a year
  - Human evaluation of pooled results returned
  - More recently other related things: Web track, HARD
- A TREC query (TREC 5)

<top>

<num> Number: 225

<desc> Description:

What is the main function of the Federal Emergency

Management Agency (FEMA) and the funding level provided to meet emergencies? Also, what resources are available to FEMA such as people, equipment, facilities?

</top>



### **Standard relevance benchmarks: Others**

#### GOV2

- Another TREC/NIST collection
- 25 million web pages
- Largest collection that is easily available
- But still 3 orders of magnitude smaller than what Google/Yahoo/MSN index
- NTCIR
  - East Asian language and cross-language information retrieval
- Cross Language Evaluation Forum (CLEF)
  - This evaluation series has concentrated on European languages and cross-language information retrieval.
- Many others



### **Text Categorization**



# **Text Classification Problem**

Given:

a set of target categories:

• the set *T* of documents,  $C = \{C^1, ..., C^n\}$ define

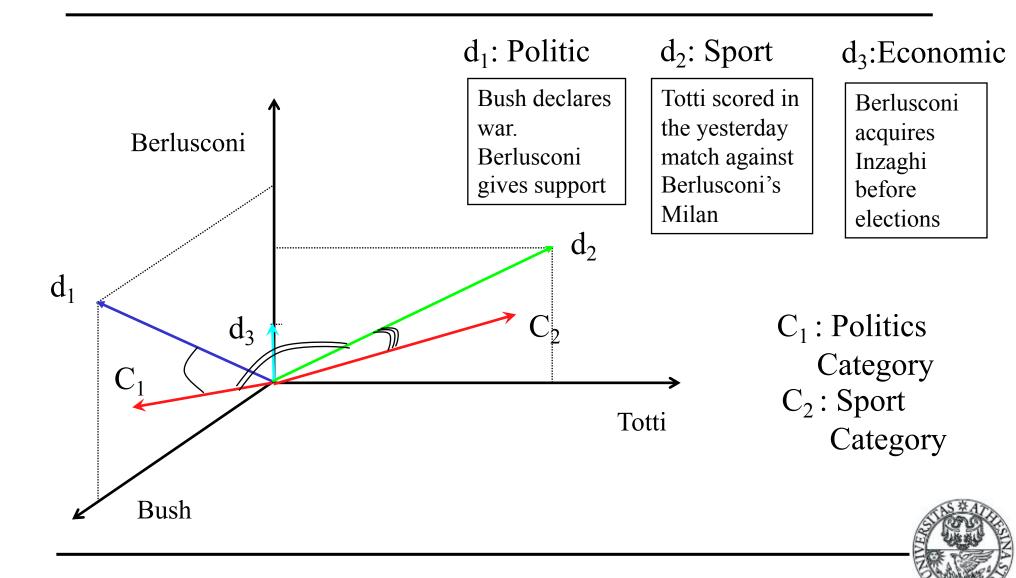
$$f: T \rightarrow 2^C$$

- VSM (Salton89')
  - Features are dimensions of a Vector Space.
  - Documents and Categories are vectors of feature weights.

• *d* is assigned to 
$$C^i$$
 if  $\vec{d} \cdot \vec{C}^i > th$ 



#### **The Vector Space Model**



#### **Automated Text Categorization**

- A corpus of pre-categorized documents
- Split document in two parts:
  - Training-set
  - Test-set
- Apply a supervised machine learning model to the training-set
  - Positive examples
  - Negative examples
- Measure the performances on the test-set
  - e.g., Precision and Recall



#### **Feature Vectors**

 Each example is associated with a vector of n feature types (e.g. unique words in TC)

 $\vec{x} = (0, ..., 1, ..., 0, ..., 0, ..., 1, ..., 0, ..., 0, ..., 1, ..., 0, ..., 1)$ acquisition buy market sell stocks

- The dot product  $\vec{X} \cdot \vec{Z}$  counts the number of features in common
- This provides a sort of similarity



# **Text Categorization phases**

- Corpus pre-processing (e.g. tokenization, stemming)
- Feature Selection (optionally)
  - Document Frequency, Information Gain, χ<sub>2</sub>, mutual information,...
- Feature weighting
  - for documents and profiles
- Similarity measure
  - between document and profile (e.g. scalar product)
- Statistical Inference
  - threshold application
- Performance Evaluation
  - Accuracy, Precision/Recall, BEP, f-measure,..



### **Feature Selection**

- Some words, i.e. features, may be irrelevant
- For example, "function words" as: "the", "on","those"...
- Two benefits:
  - efficiency
  - Sometime the accuracy
- Sort features by relevance and select the *m*-best



## **Statistical Quantity to sort feature**

#### Based on corpus counts of the pair

- A is the number of documents in which both f and c occur, i.e. (f, c);
- B is the number of documents in which only f occurs, i.e.  $(f, \bar{c})$ ;
- C is the number of documents in which only c occurs, i.e.  $(\bar{f}, c)$ ;
- *D* is the number of documents in which neither *f* nor *c* occur, i.e.  $(\bar{f}, \bar{c})$ ;
- N is the total number of documents, i.e. A + B + C + D.



#### Chi-square, Pointwise MI and MI

$$\begin{split} \chi^2(f,c) &= \frac{N \times (AD - CB)^2}{(A + C)(B + D)(A + B)(C + D)} \\ PMI(f,c) &= \log \frac{P(f,c)}{P(f) \times P(c)} \\ MI(f) &= -\sum_{c \in \mathcal{C}} P(c) log(P(c)) + P(f) \sum_{c \in \mathcal{C}} P(c|f) log(P(c|f)) \\ &+ P(\bar{f}) \sum_{c \in \mathcal{C}} P(c|\bar{f}) log(P(c|\bar{f})) \end{split}$$



# Profile Weighting: the Rocchio's formula

- $\omega_f^d$ , the weight of f in d
  - Several weighting schemes (e.g. TF \* IDF, Salton 91')
- $\vec{C}_{f}^{i}$ , the profile weights of f in  $C_{i}$ :

$$\vec{C}_{f}^{i} = \max\left\{ 0, \frac{\beta}{|T_{i}|} \sum_{d \in T_{i}} \omega_{f}^{d} - \frac{\gamma}{|\overline{T}_{i}|} \sum_{d \in \overline{T}_{i}} \omega_{f}^{d} \right\}$$

•  $T_i$ , the training documents in  $C^i$ 



# **Similarity estimation**

Given the document and the category representation

$$\vec{d} = \langle \omega_{f_1}^d, ..., \omega_{f_n}^d \rangle, \quad \vec{C}_i = \langle \Omega_{f_1}^i, ..., \Omega_{f_n}^i \rangle$$

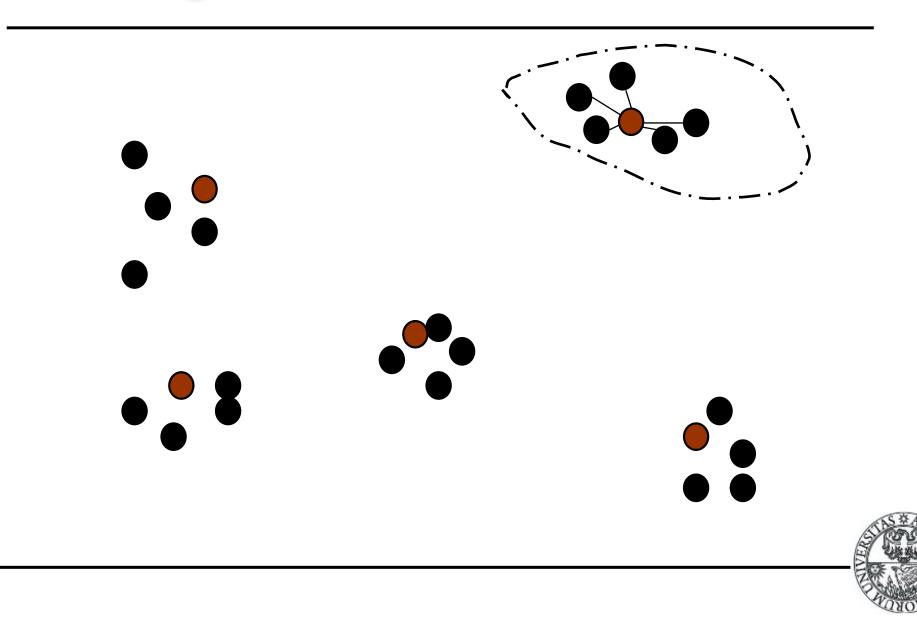
It can be defined the following similarity function (cosine measure

$$s_{d,i} = \cos(\vec{d} \ , \vec{C}_i) = \frac{\vec{d} \cdot \vec{C}^i}{\left\|\vec{d} \ \| \times \|\vec{C}_i\|} = \frac{\sum_{f} \omega_f^d \times \Omega_f^i}{\left\|\vec{d} \ \| \times \|\vec{C}_i\|}$$

• *d* is assigned to  $C^i$  if  $\vec{d} \cdot \vec{C}^i > \sigma$ 



# Clustering



# **Experiments**

Reuters Collection 21578 Apté split (Apté94)

- 90 classes (12,902 docs)
- A fixed splitting between training and test set
- 9603 vs 3299 documents
- Tokens
  - about 30,000 different
- Other different versions have been used but ...

most of TC results relate to the 21578 Apté

 [Joachims 1998], [Lam and Ho 1998], [Dumais et al. 1998], [Li Yamanishi 1999], [Weiss et al. 1999],
 [Cohen and Singer 1999]...



# **A Reuters document- Acquisition Category**

CRA SOLD FORREST GOLD FOR 76 MLN DLRS - WHIM CREEK

SYDNEY, April 8 - <Whim Creek Consolidated NL> said the consortium it is leading will pay 76.55 mln dlrs for the acquisition of CRA Ltd's <CRAA.S> <Forrest Gold Pty Ltd> unit, reported yesterday.

CRA and Whim Creek did not disclose the price yesterday.

Whim Creek will hold 44 pct of the consortium, while

<Austwhim Resources NL> will hold 27 pct and <Croesus Mining NL> 29 pct, it said in a statement.

As reported, Forrest Gold owns two mines in Western Australia producing a combined 37,000 ounces of gold a year. It also owns an undeveloped gold project.



# A Reuters document- Crude-Oil Category

#### FTC URGES VETO OF GEORGIA GASOLINE STATION BILL

WASHINGTON, March 20 - The Federal Trade Commission said its staff has urged the governor of Georgia to veto a bill that would prohibit petroleum refiners from owning and operating retail gasoline stations.

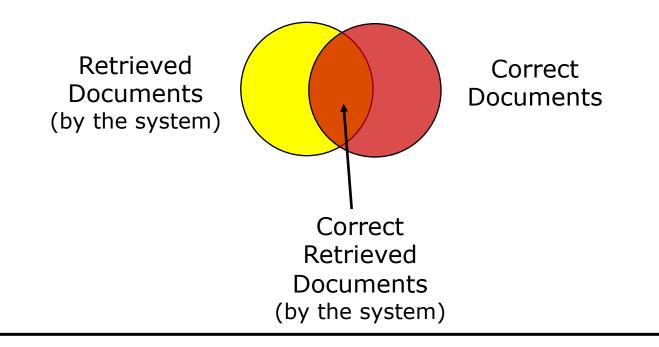
The proposed legislation is aimed at preventing large oil refiners and marketers from using predatory or monopolistic practices against franchised dealers.

But the FTC said fears of refiner-owned stations as part of a scheme of predatory or monopolistic practices are unfounded. It called the bill anticompetitive and warned that it would force higher gasoline prices for Georgia motorists.



# **Performance Measurements**

- Given a set of document T
- Precision = # Correct Retrieved Document / # Retrieved Documents
- Recall = # Correct Retrieved Document/ # Correct Documents





### **Precision and Recall of C**<sub>i</sub>

- a, corrects
- b, mistakes

The Precision and Recall are defined by the above counts:

$$Precision_i = \frac{a_i}{a_i + b_i}$$
$$Recall_i = \frac{a_i}{a_i + c_i}$$



# Performance Measurements (cont'd)

- Breakeven Point
  - Find thresholds for which Recall = Precision
  - Interpolation
- f-measure
  - Harmonic mean between precision and recall
- Global performance on more than two categories
  - Micro-average
    - The counts refer to classifiers
  - Macro-average (average measures over all categories)



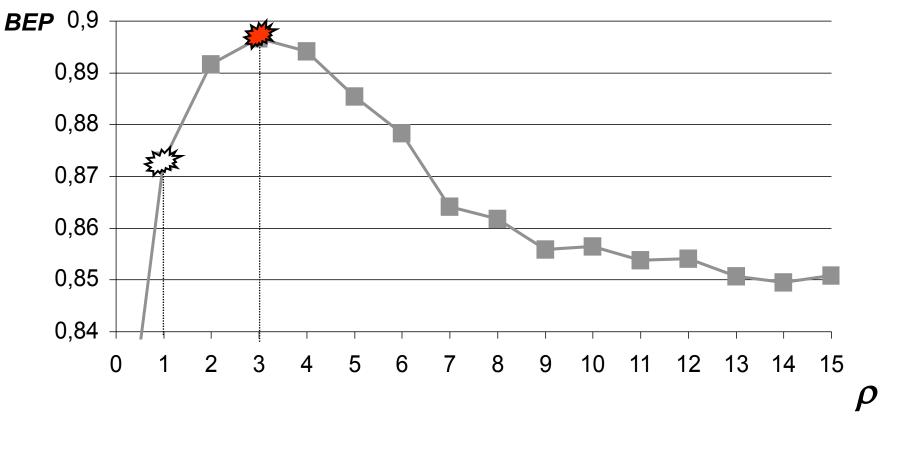
#### **F-measure e MicroAverages**

$$F_{1} = \frac{2 \times Precision \times Recall}{Precision + Recall}$$
$$\mu Precision = \frac{\sum_{i=1}^{n} a_{i}}{\sum_{i=1}^{n} a_{i} + b_{i}}$$
$$\mu Recall = \frac{\sum_{i=1}^{n} a_{i}}{\sum_{i=1}^{n} a_{i} + c_{i}}$$
$$\mu BEP = \frac{\mu Precision + \mu Recall}{2}$$

$$\mu f_1 = \frac{2 \times \mu Precision \times \mu Recall}{\mu Precision + \mu Recall}$$

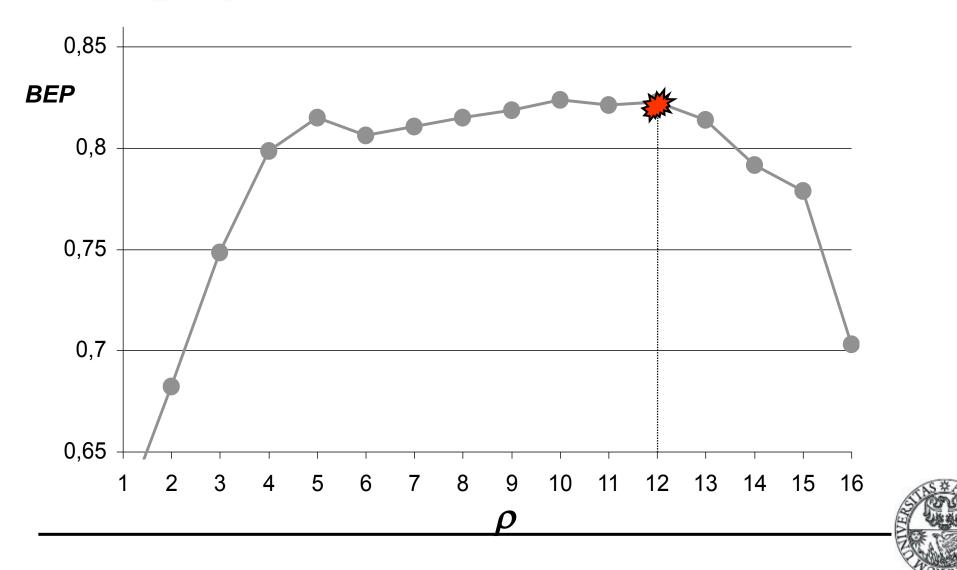


# The Impact of $\rho$ parameter on Acquisition category





# The impact of $\rho$ parameter on Trade category



### **N-fold cross validation**

- Divide training set in n parts
  - One is used for testing
  - *n-1* for training
- This can be repeated *n* times for *n* distinct test sets
- Average and Std. Dev. are the final performance index



# **Introduction to Machine Learning**

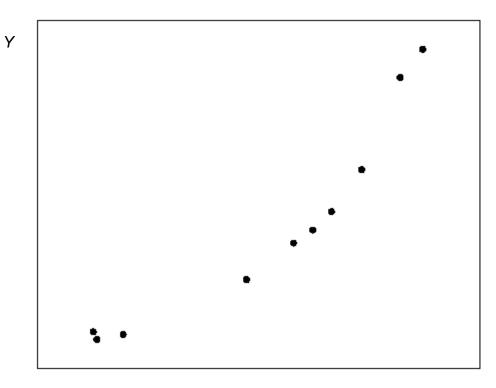


# What is Statistical Learning?

- Statistical Methods Algorithms that learn relations in the data from examples
- Simple relations are expressed by pairs of variables:  $\langle x_1, y_1 \rangle$ ,  $\langle x_2, y_2 \rangle$ ,...,  $\langle x_n, y_n \rangle$
- Learning *f* such that evaluate  $y^*$  given a new value  $x^*$ , i.e.  $\langle x^*, f(x^*) \rangle = \langle x^*, y^* \rangle$

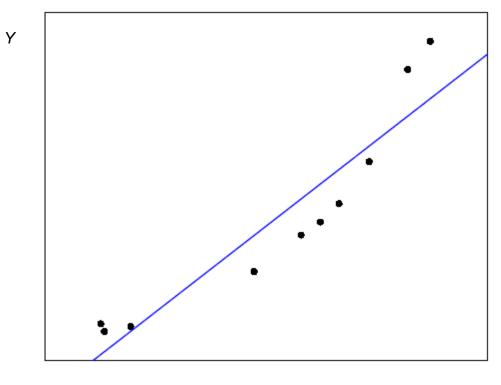


# You have already tackled the learning problem



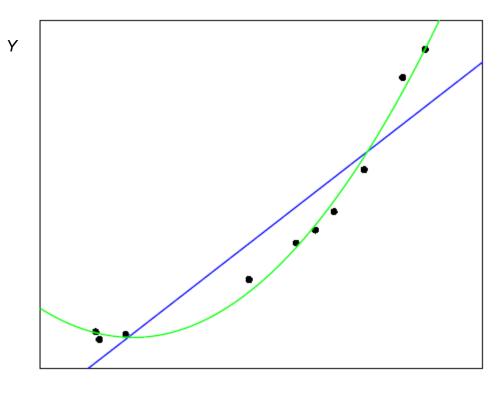


#### **Linear Regression**



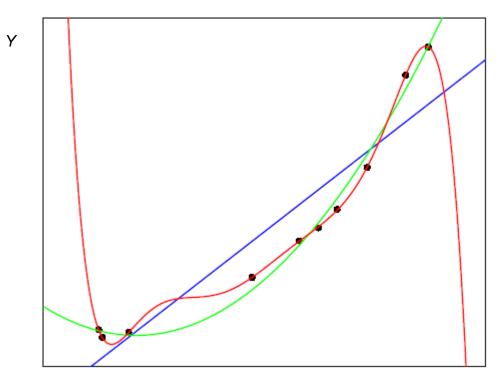


### Degree 2





#### Degree





# **Machine Learning Problems**

- Overfitting
- How dealing with millions of variables instead of only two?
- How dealing with real world objects instead of real values?



# **Linear Classifiers**



# Linear Classifier (1)

• The equation of a hyperplane is

$$f(\vec{x}) = \vec{x} \cdot \vec{w} + b = 0, \quad \vec{x}, \vec{w} \in \Re^n, b \in \Re$$

- $\vec{x}$  is the vector representing the classifying example
- $\vec{w}$  is the gradient to the hyperplane

The classification function is

 $h(x) = \operatorname{sign}(f(x))$ 

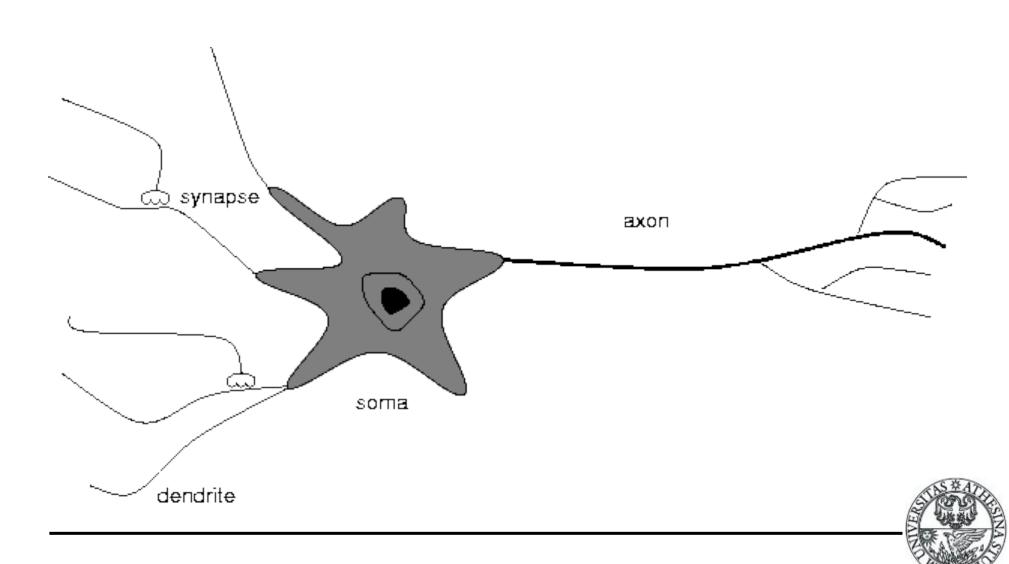


# Linear classifiers (2)

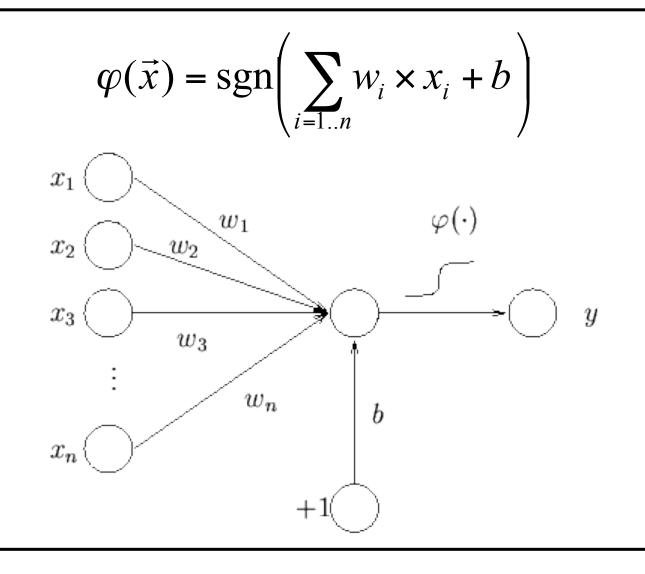
- Linear Functions are the simplest ones from an analytical point of view.
- The basic idea is to select a hypothesis with null error on the training-set.
- To learn a linear function a simple neural network of only one neuron is enough (Perceptron)



### An animal neuron



# **The Perceptron**





- Functional Margin of an example with respect to a hyperplane:  $\gamma_i = y_i(\vec{w} \cdot \vec{x}_i + b)$
- The distribution of functional margins of a hyperplane with respect to a training set *S* is the distribution of the margins of the examples  $in(\mathfrak{B}, \mathfrak{W})t$ the hyperplane .
- The functional margin of a hyperplane is the minimum margin of the distribution



# Notations (con'td)

If we normalize the hyperplane equation, i.e.

 $\left(\frac{\vec{w}}{\|\vec{w}\|}, \frac{b}{\|\vec{w}\|}\right)$ , we obtain the **geometric margin** 

- The *geometric margin* measure the Euclidean distance between the target point and the hyperplane.
- The training set Margin is the maximum geometric (functional) margin among all hyperplanes which separates the examples in S.
- The hyperplane associated with the above quantity is called maximal margin hyperplane



#### **Basic Concepts**

From 
$$\cos(\vec{x}, \vec{w}) = \frac{\vec{x} \cdot \vec{w}}{\|\vec{x}\| \cdot \|\vec{w}\|}$$

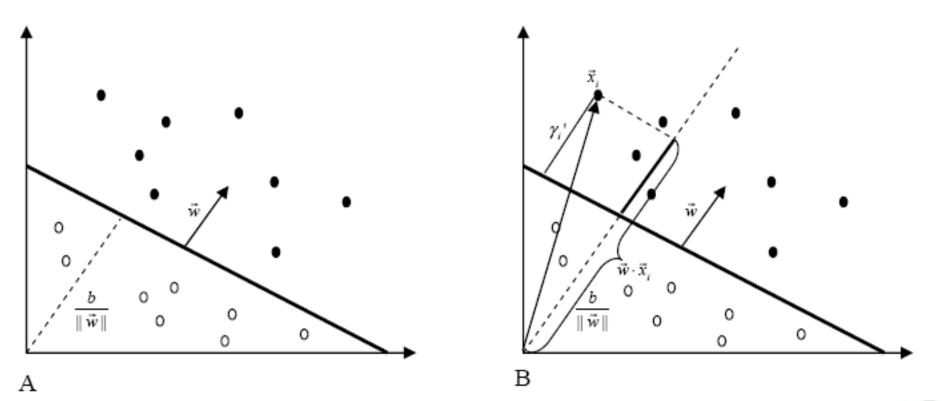
It follows that

$$\|\vec{x}\|\cos(\vec{x},\vec{w}) = \frac{\vec{x}\cdot\vec{w}}{\|\vec{w}\|} = \vec{x}\cdot\frac{\vec{w}}{\|\vec{w}\|}$$

Norm of  $\operatorname{tim}_{\mathcal{X}}$  s the cosine between and , i.e. the  $\operatorname{pr}_{\mathcal{X}}$  jection of  $\mathcal{W}$  on  $\vec{X} \quad \vec{\mathcal{W}}$ 

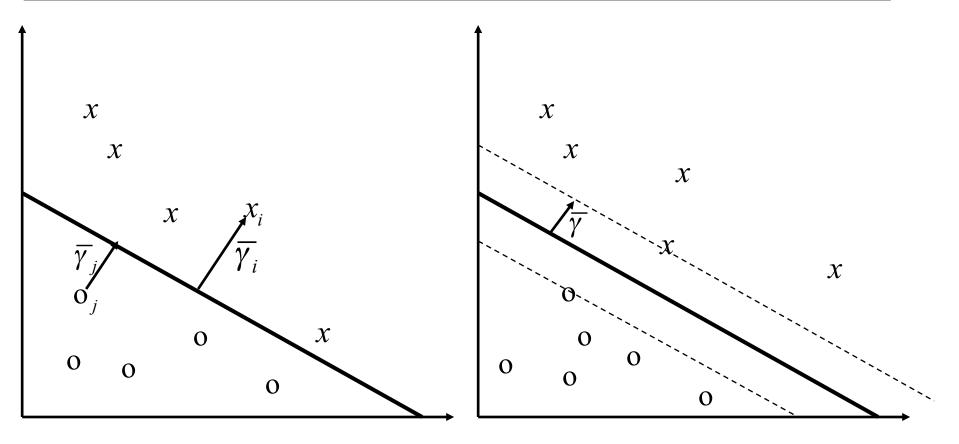


# **Geometric Margin**





# Geometric margins of 2 points and hyperplane margin

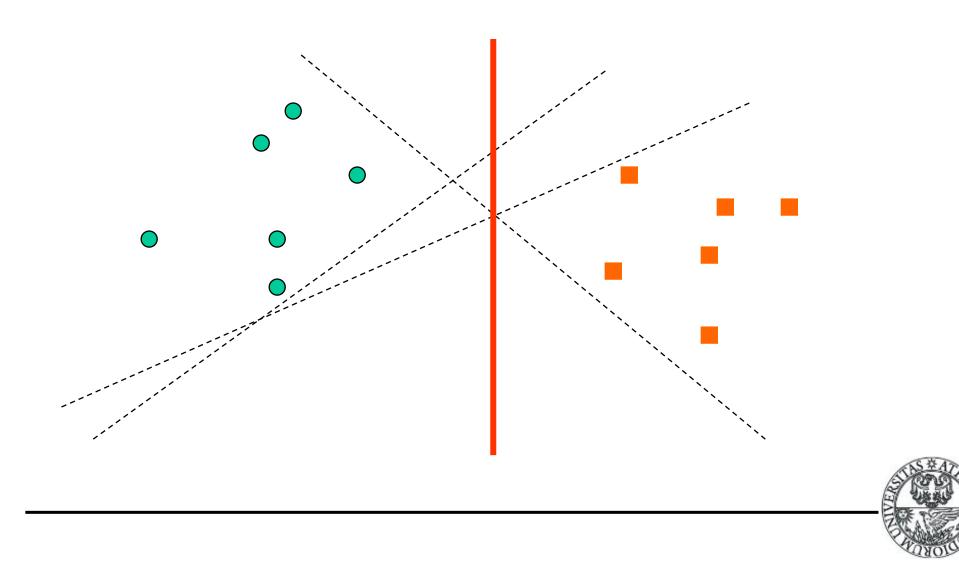


Geometric Margin

Hyperplane Margin



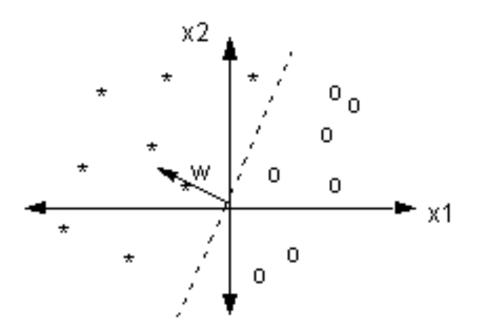
#### Maximal margin vs other margins



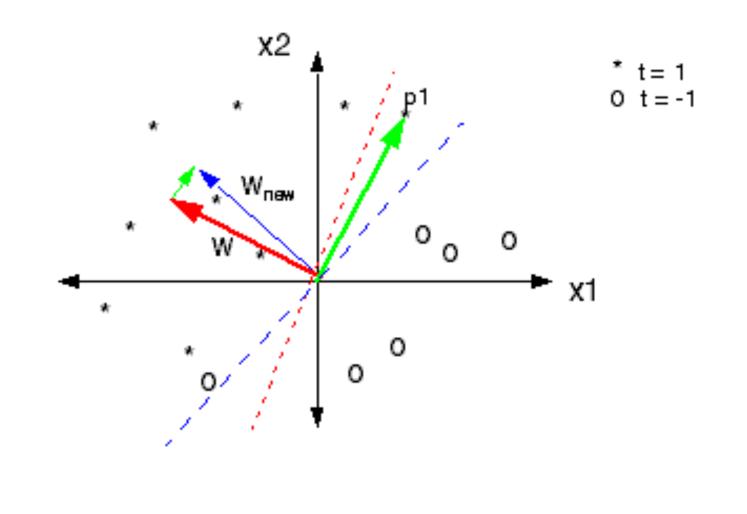
# Perceptron training on a data set (on-line algorthm)

$$\vec{w}_{0} \leftarrow \vec{0}; b_{0} \leftarrow 0; k \leftarrow 0; R \leftarrow \max_{1 \le i \le l} || \vec{x}_{i} ||$$
Repeat  
for i = 1 to m  
if  $y_{i}(\vec{w}_{k} \cdot \vec{x}_{i} + b_{k}) \le 0$  then  
 $\vec{w}_{k+1} = \vec{w}_{k} + \eta y_{i} \vec{x}_{i}$   
 $b_{k+1} = b_{k} + \eta y_{i} R^{2}$   
 $k = k + 1$   
endif  
endfor  
until no error is found  
return  $k, (\vec{w}_{k}, b_{k})$ 

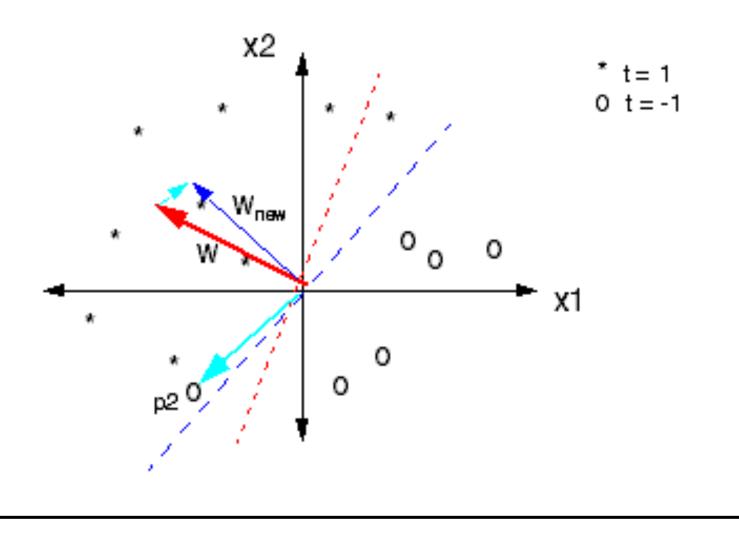




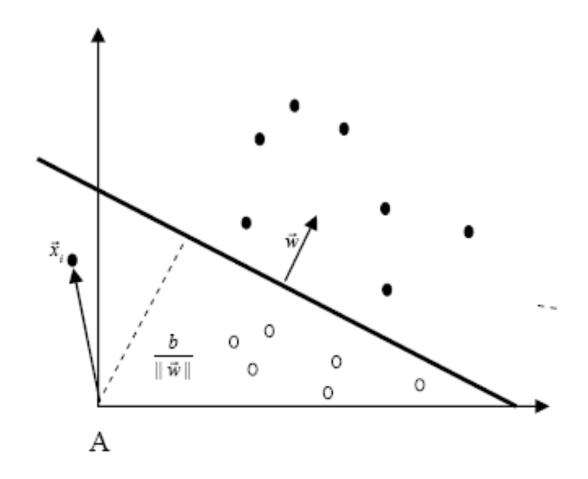




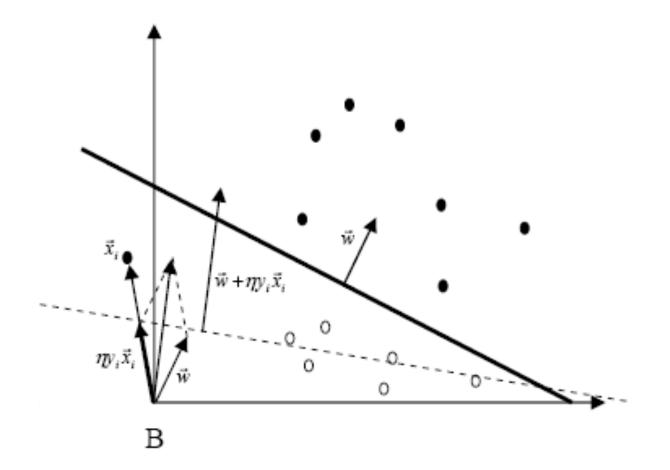




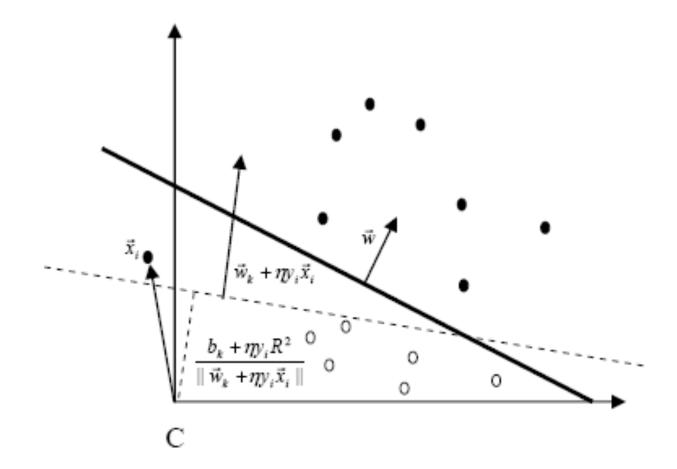














Let *S* be a non-trivial training-set and let

$$R = \max_{i=1,\dots,m} || x_i ||.$$

Let us suppose there is a vector  $\mathbf{w}^*$ ,  $||\mathbf{w}^*||=1$  and

$$y_i(\langle \mathbf{w}^*, \mathbf{x}_i \rangle + b^*) \ge \gamma, \quad i = 1,..,m,$$

with  $\gamma > 0$ . Then the maximum number of errors of the perceptron is:

$$t^* = \left(\frac{2R}{\gamma}\right)^2,$$



# **Observations**

- The theorem states that independently of the margin size, if data is linearly separable the perceptron algorithm finds the solution in a finite amount of steps.
- This number is inversely proportional to the square of the margin.
- The bound is invariant with respect to the scale of the patterns (i.e. only the relative distances count).
- The learning rate is not essential for the convergence.



# **Dual Representation**

The decision function can be rewritten as:

$$h(x) = \operatorname{sgn}(\vec{w} \cdot \vec{x} + b) = \operatorname{sgn}(\sum_{j=1..m} \alpha_j y_j \vec{x}_j \cdot \vec{x} + b) =$$
  
$$\operatorname{sgn}(\sum_{i=1..m} \alpha_j y_j \vec{x}_j \cdot \vec{x} + b)$$

• as well as the updating function

if 
$$y_i (\sum_{j=1..m} \alpha_j y_j \vec{x}_j \cdot \vec{x}_i + b) \le 0$$
 then  $\alpha_i = \alpha_i + \eta$ 

• The learning rate  $\eta$  only affects the re-scaling of the hyperplane, it does not affect the algorithm, so we can fix  $\eta = 1$ .



# **First properties of SVMs**

DUALITY is the first feature of Support Vector Machines
SVMs are learning machines using the following function:

$$f(x) = \operatorname{sgn}(\vec{w} \cdot \vec{x} + b) = \operatorname{sgn}(\sum_{j=1..m} \alpha_j y_j \vec{x}_j \cdot \vec{x} + b)$$

- Note that data appears only as scalar product (for both testing and learning phases)
- The Matrix  $G = (\vec{x}_i \cdot \vec{x}_j)_{i,j=1}^m$  is called Gram matrix



- Data must be linearly separable
- Noise (almost all classifier types)
- Data must be in vectorial format



# Solutions

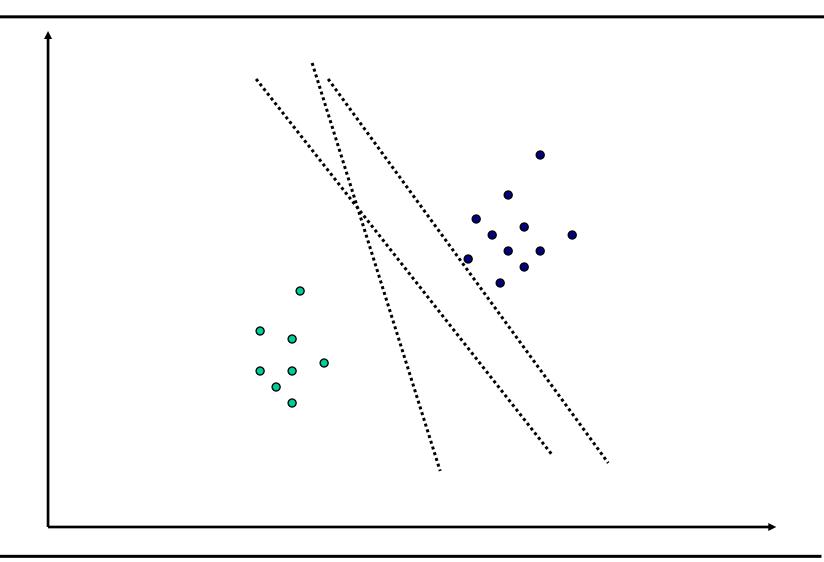
- Multi-Layers Neural Network: back-propagation learning algorithm.
- **SVMs**: kernel methods.
  - The learning algorithm is decoupled by the application domain which is encoded by a kernel function



# **Support Vector Machines**

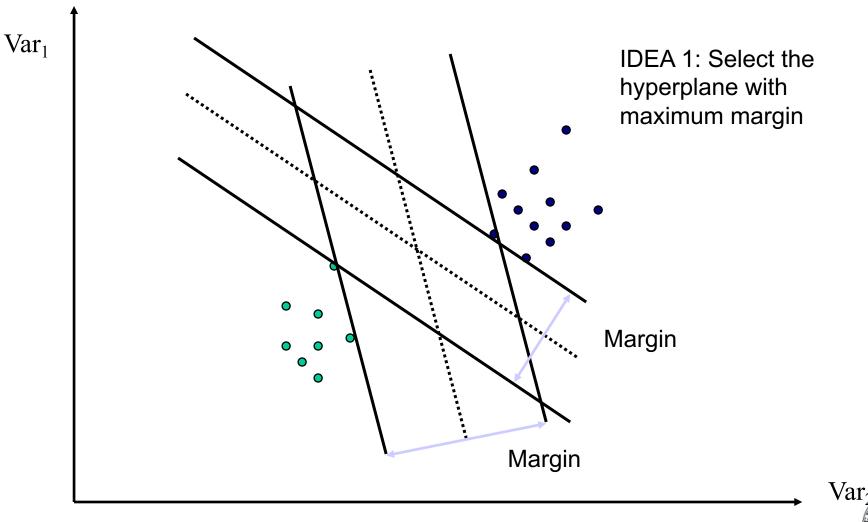


## Which hyperplane choose?



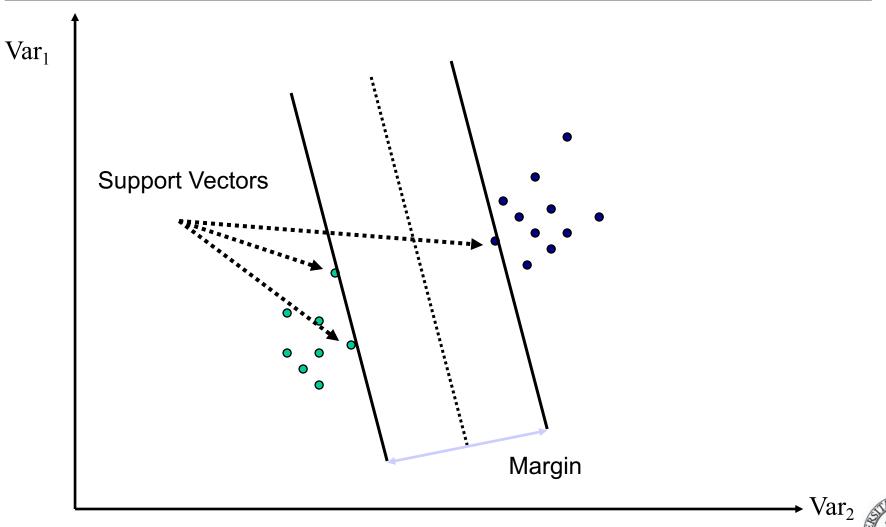


# **Classifier with a Maximum Margin**



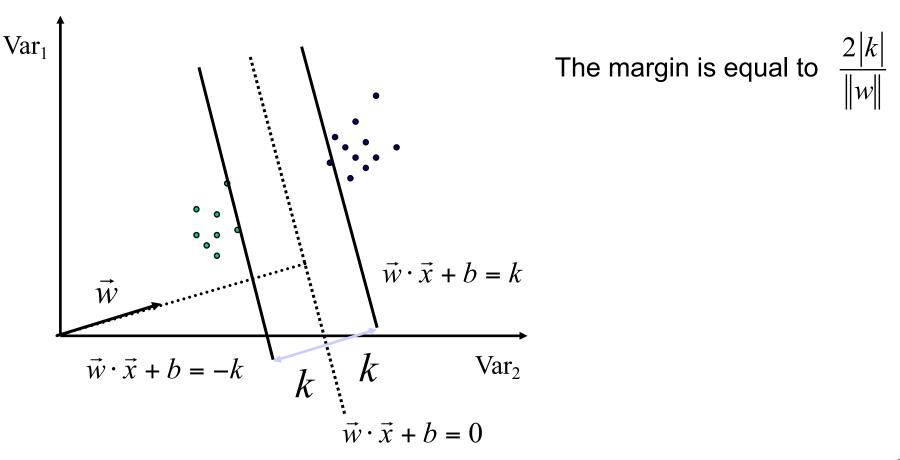


# **Support Vector**



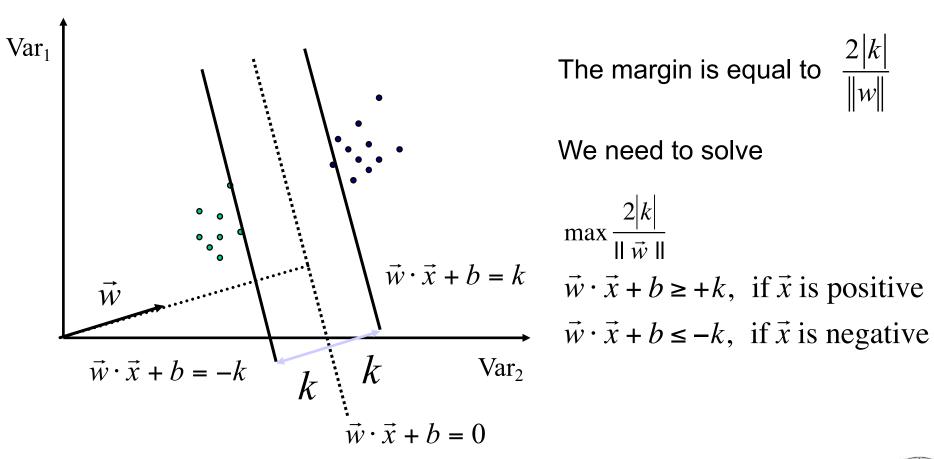


# **Support Vector Machine Classifiers**



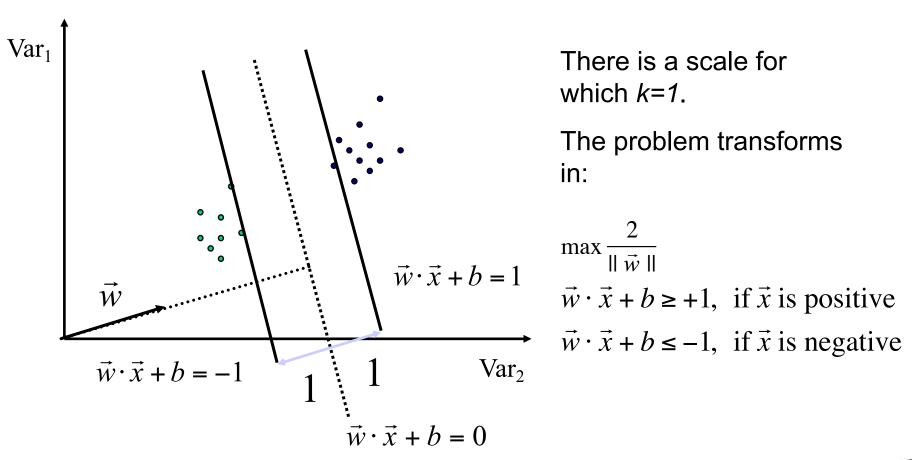


# **Support Vector Machines**





# **Support Vector Machines**





#### **Final Formulation**

$$\max \frac{2}{\|\vec{w}\|} \qquad \Rightarrow \qquad \max \frac{2}{\|\vec{w}\|} \qquad \Rightarrow \qquad \max \frac{2}{\|\vec{w}\|} \qquad \Rightarrow \qquad \\ \vec{w} \cdot \vec{x}_i + b \ge +1, \ y_i = 1 \qquad \Rightarrow \qquad y_i(\vec{w} \cdot \vec{x}_i + b) \ge 1 \qquad \end{aligned}$$

$$\Rightarrow \min \frac{\|\vec{w}\|}{2} \Rightarrow \min \frac{\|\vec{w}\|^2}{2}$$
$$y_i(\vec{w} \cdot \vec{x}_i + b) \ge 1 \qquad y_i(\vec{w} \cdot \vec{x}_i + b) \ge 1$$



# **Optimization Problem**

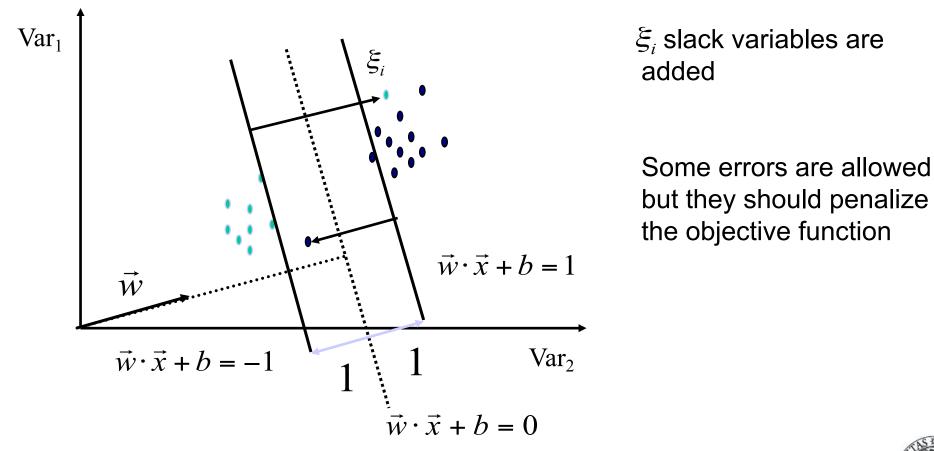
Optimal Hyperplane:

• Minimize 
$$\tau(\vec{w}) = \frac{1}{2} \|\vec{w}\|^2$$

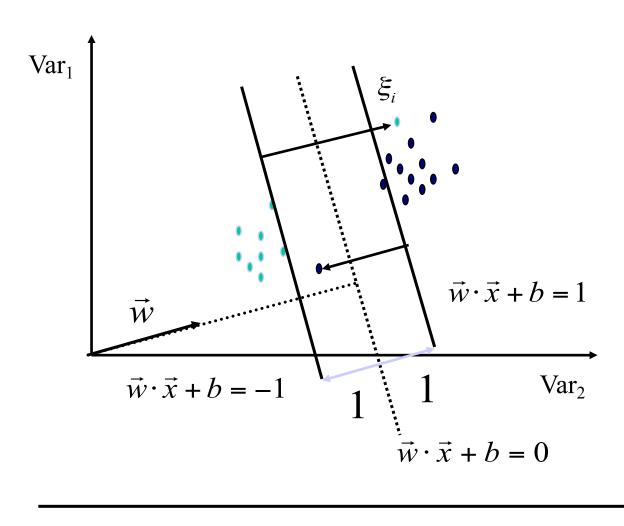
■ Subject to 
$$y_i ((\vec{w} \cdot \vec{x}_i) + b) \ge 1, i = 1, ..., m$$

The dual problem is simpler









The new constraints are

$$y_i(\vec{w} \cdot \vec{x}_i + b) \ge 1 - \xi_i$$
  
 
$$\forall \vec{x}_i \text{ where } \xi_i \ge 0$$

The objective function penalizes the incorrect classified examples

$$\min\frac{1}{2} \|\vec{w}\|^2 + C\sum_i \xi_i$$

C is the trade-off between margin and the error



#### **Dual formulation**

$$\begin{cases} \min \quad \frac{1}{2} ||\vec{w}|| + C \sum_{i=1}^{m} \xi_i^2 \\ y_i(\vec{w} \cdot \vec{x_i} + b) \ge 1 - \xi_i, \quad \forall i = 1, ..., m \\ \xi_i \ge 0, \quad i = 1, ..., m \end{cases}$$

$$L(\vec{w}, b, \vec{\xi}, \vec{\alpha}) = \frac{1}{2}\vec{w} \cdot \vec{w} + \frac{C}{2}\sum_{i=1}^{m} \xi_i^2 - \sum_{i=1}^{m} \alpha_i [y_i(\vec{w} \cdot \vec{x_i} + b) - 1 + \xi_i],$$

• By deriving wrt  $\vec{w}, \vec{\xi}$  and b



#### **Final dual optimization problem**

$$\sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \left( \vec{x_i} \cdot \vec{x_j} + \frac{1}{C} \delta_{ij} \right)$$
$$\alpha_i \ge 0, \quad \forall i = 1, ..., m$$
$$\sum_{i=1}^{m} y_i \alpha_i = 0$$



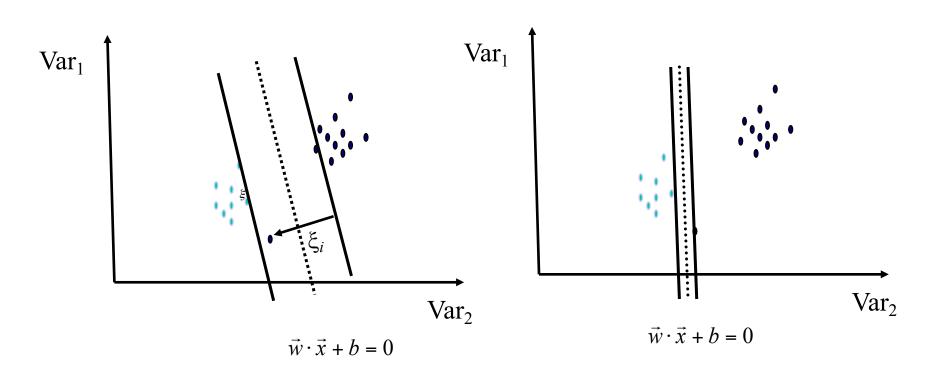
# **Soft Margin Support Vector Machines**

$$\min \frac{1}{2} \| \vec{w} \|^2 + C \sum_i \xi_i \qquad \begin{array}{l} y_i (\vec{w} \cdot \vec{x}_i + b) \ge 1 - \xi_i \quad \forall \vec{x}_i \\ \xi_i \ge 0 \end{array}$$

- The algorithm tries to keep  $\xi_i$  low and maximize the margin
- NB: The number of error is not directly minimized (NP-complete problem); the distances from the hyperplane are minimized
- If  $C \rightarrow \infty$ , the solution tends to the one of the *hard-margin* algorithm
- Attention !!!: if C = 0 we get  $\|\vec{w}\| = 0$ , since  $y_i b \ge 1 \xi_i$   $\forall \vec{x}_i$
- If C increases the number of error decreases. When C tends to infinite the number of errors must be 0, i.e. the *hard-margin* formulation



#### Robusteness of Soft vs. Hard Margin SVMs





Hard Margin SVM



# **Soft vs Hard Margin SVMs**

- *Soft-Margin* has ever a solution
- Soft-Margin is more robust to odd examples
- *Hard-Margin* does not require parameters



## **Parameters**

$$\min \frac{1}{2} \| \vec{w} \|^{2} + C \sum_{i} \xi_{i} = \min \frac{1}{2} \| \vec{w} \|^{2} + C^{+} \sum_{i} \xi_{i}^{+} + C^{-} \sum_{i} \xi_{i}^{-}$$
$$= \min \frac{1}{2} \| \vec{w} \|^{2} + C \left( J \sum_{i} \xi_{i}^{+} + \sum_{i} \xi_{i}^{-} \right)$$

- C: trade-off parameter
- J: cost factor



# **Kernel Methods**

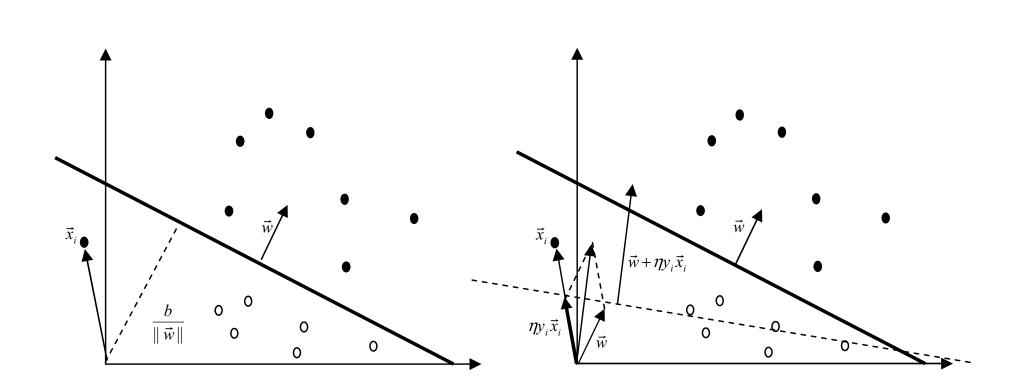


# An example of kernel-based machine: Perceptron training

 $\vec{w}_0 \leftarrow \vec{0}; b_0 \leftarrow 0; k \leftarrow 0; R \leftarrow \max_{1 \le i \le l} \|\vec{x}_i\|$ do for i = 1 to  $\ell$ if  $y_i(\vec{w}_k \cdot \vec{x}_i + b_k) \le 0$  then  $\vec{w}_{k+1} = \vec{w}_k + \eta y_i \vec{x}_i$  $b_{k+1} = b_k + \eta y_k R^2$ k = k + 1endif endfor while an error is found return k,  $(\vec{w}_k, b_k)$ 



# **Graphic interpretation of the Perceptron**





# **Dual Representation for Classification**

In each step of perceptron algorithm only training data is added with a certain weight:

$$\vec{w} = \sum_{j=1..\ell} \alpha_j y_j \vec{x}_j$$

Hence the classification function results:

$$\operatorname{sgn}(\vec{w} \cdot \vec{x} + b) = \operatorname{sgn}\left(\sum_{j=1..\ell} \alpha_j y_j \vec{x}_j \cdot \vec{x} + b\right)$$

Note that data only appears in the scalar product



# **Dual Representation for Learning**

as well as the updating function

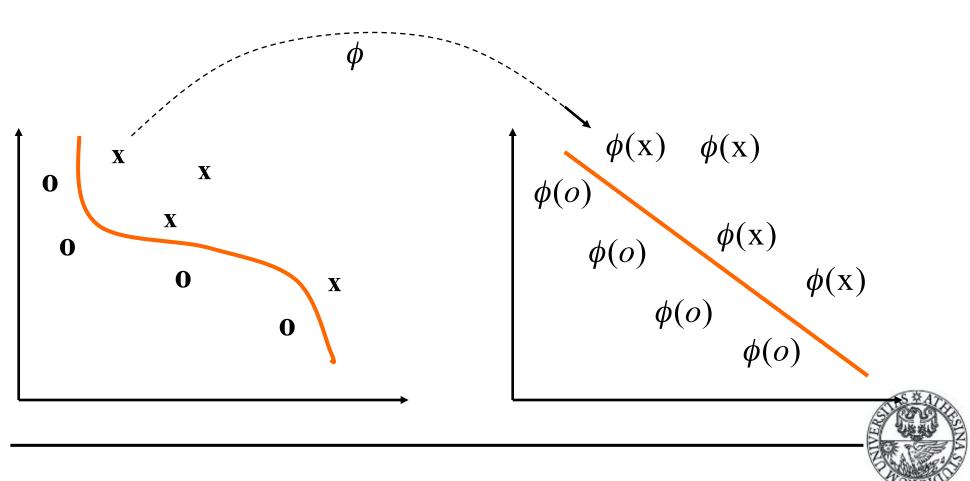
$$\text{if } y_i \left( \sum_{j=1..\ell} \alpha_j y_j \vec{x}_j \cdot \vec{x}_i + b \right) \le 0 \text{ then } \alpha_i = \alpha_i + \eta$$

The learning rate  $\eta$  only affects the re-scaling of the hyperplane, it does not affect the algorithm, so we can fix  $\eta = 1$ 



# **The main idea of Kernel Functions**

• Mapping vectors in a space where they are linearly separable,  $\vec{x} \rightarrow \phi(\vec{x})$ 



## **Soft Margin optimization problem**

$$\begin{array}{ll} maximize & \sum_{i=1}^{m} \alpha_{i} - \frac{1}{2} \sum_{i,j=1}^{m} y_{i} y_{j} \alpha_{i} \alpha_{j} \left( \vec{x_{i}} \cdot \vec{x_{j}} + \frac{1}{C} \delta_{ij} \right) \\ subject \ to & \alpha_{i} \geq 0, \quad \forall i = 1, ..., m \\ & \sum_{i=1}^{m} y_{i} \alpha_{i} = 0 \end{array}$$



## **Kernels in Support Vector Machines**

In Soft Margin SVMs we maximize:

$$\sum_{i=1}^{m} \alpha_{i} - \frac{1}{2} \sum_{i,j=1}^{m} y_{i} y_{j} \alpha_{i} \alpha_{j} \left( \boldsymbol{x}_{i} \cdot \boldsymbol{x}_{j} + \frac{1}{C} \delta_{ij} \right)$$

By using kernel functions we rewrite the problem as:

$$\begin{cases} maximize \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \left( k(o_i, o_j) + \frac{1}{C} \delta_{ij} \right) \\ \alpha_i \ge 0, \quad \forall i = 1, ..., m \\ \sum_{i=1}^{m} y_i \alpha_i = 0 \end{cases}$$



## **Kernel Function Definition**

**Def. 2.26** A kernel is a function k, such that  $\forall \vec{x}, \vec{z} \in X$ 

$$k(\vec{x}, \vec{z}) = \boldsymbol{\phi}(\vec{x}) \cdot \boldsymbol{\phi}(\vec{z})$$

where  $\phi$  is a mapping from X to an (inner product) feature space.

Kernels are the product of mapping functions such as

$$\vec{x} \in \Re^n$$
,  $\vec{\phi}(\vec{x}) = (\phi_1(\vec{x}), \phi_2(\vec{x}), \dots, \phi_m(\vec{x})) \in \Re^m$ 



## **The Kernel Gram Matrix**

The <u>sole</u> information used for training is the kernel Gram matrix

$$K_{training} = \begin{bmatrix} k(\mathbf{x}_{1}, \mathbf{x}_{1}) & k(\mathbf{x}_{1}, \mathbf{x}_{2}) & \dots & k(\mathbf{x}_{1}, \mathbf{x}_{m}) \\ k(\mathbf{x}_{2}, \mathbf{x}_{1}) & k(\mathbf{x}_{2}, \mathbf{x}_{2}) & \dots & k(\mathbf{x}_{2}, \mathbf{x}_{m}) \\ \dots & \dots & \dots & \dots \\ k(\mathbf{x}_{m}, \mathbf{x}_{1}) & k(\mathbf{x}_{m}, \mathbf{x}_{2}) & \dots & k(\mathbf{x}_{m}, \mathbf{x}_{m}) \end{bmatrix}$$

If the kernel is valid, K is symmetric positive-semidefinite



## Valid Kernels

**Def. B.11** Eigen Values Given a matrix  $A \in \mathbb{R}^m \times \mathbb{R}^n$ , an egeinvalue  $\lambda$  and an egeinvector  $\vec{x} \in \mathbb{R}^n - {\vec{0}}$  are such that

$$A\vec{x} = \lambda\vec{x}$$

**Def. B.12** Symmetric Matrix A square matrix  $A \in \mathbb{R}^n \times \mathbb{R}^n$  is symmetric iff  $A_{ij} = A_{ji}$  for  $i \neq j$  i = 1, ..., mand j = 1, ..., n, i.e. iff A = A'.

**Def. B.13** Positive (Semi-) definite Matrix A square matrix  $A \in \mathbb{R}^n \times \mathbb{R}^n$  is said to be positive (semi-) definite if its eigenvalues are all positive (non-negative).



## Valid Kernels cont'd

**Proposition 1.** (Mercer's conditions)

Let X be a finite input space and let  $K(\mathbf{x}, \mathbf{z})$  be a symmetric function on X. Then  $K(\mathbf{x}, \mathbf{z})$  is a kernel function if and only if the matrix

 $k(\boldsymbol{x},\boldsymbol{z}) = \boldsymbol{\phi}(\boldsymbol{x}) \cdot \boldsymbol{\phi}(\boldsymbol{z})$ 

is positive semi-definite (has non-negative eigenvalues).

If the matrix is positive semi-definite then we can find a mapping  $\phi$  implementing the kernel function



■ It may not be a kernel so we can use **M**′·**M** 

**Proposition B.14** Let A be a symmetric matrix. Then A is positive (semi-) definite iff for any vector  $\vec{x} \neq 0$ 

$$\vec{x}' A \vec{x} > \lambda \vec{x} \quad (\geq 0).$$

From the previous proposition it follows that: If we find a decomposition A in M'M, then A is semi-definite positive matrix as

$$\vec{x}' \mathbf{A} \vec{x} = \vec{x}' \mathbf{M}' \mathbf{M} \vec{x} = (\mathbf{M} \vec{x})' (\mathbf{M} \vec{x}) = \mathbf{M} \vec{x} \cdot \mathbf{M} \vec{x} = ||\mathbf{M} \vec{x}||^2 \ge 0.$$



## **Valid Kernel operations**

- $k(x,z) = k_1(x,z) + k_2(x,z)$
- $k(x,z) = k_1(x,z)^*k_2(x,z)$
- $k(x,z) = \alpha k_1(x,z)$
- k(x,z) = f(x)f(z)
- k(x,z) = x'Bz
- $k(x,z) = k_1(\phi(x),\phi(z))$



## **Object Transformation** [Moschitti et al, CLJ 2008]

$$K(O_1, O_2) = \phi(O_1) \cdot \phi(O_2) = \phi_E(\phi_M(O_1)) \cdot \phi_E(\phi_M(O_2))$$
  
=  $\phi_E(S_1) \cdot \phi_E(S_2) = K_E(S_1, S_2)$ 

#### • Canonical Mapping, $\phi_{M}()$

- object transformation,
- e. g., a syntactic parse tree into a verb subcategorization frame tree.

#### • Feature Extraction, $\phi_{E}()$

- maps the canonical structure in all its fragments
- different fragment spaces, e.g. String and Tree Kernels



### Part I – Basic Kernels (for structured data)

Basic Kernels and their Feature Spaces (35 min)

- Linear Kernels
- Polynomial Kernels
- Lexical Semantic Kernels
- String and Word Sequence Kernels
- Syntactic Tree Kernel, Partial Tree kernel (PTK), Semantic Syntactic Tree Kernel, Smoothed PTK

## Linear Kernel

In Text Categorization documents are word vectors

$$\Phi(d_x) = \vec{x} = (0, ..., 1, ..., 0, ..., 0, ..., 1, ..., 0, ..., 0, ..., 1, ..., 0, ..., 1)$$
  
buy market sell stocks trade  
$$\Phi(d_z) = \vec{z} = (0, ..., 1, ..., 0, ..., 0, ..., 0, ..., 1, ..., 0, ..., 0, ..., 1, ..., 0, ..., 0)$$
  
buy company sell stock

- The dot product  $\vec{x} \cdot \vec{z}$  counts the number of features in common
- This provides a sort of *similarity*



## Feature Conjunction (polynomial kernel)

The initial vectors are mapped in a higher space

$$\Phi(\langle x_1, x_2 \rangle) \to (x_1^2, x_2^2, \sqrt{2}x_1 x_2, \sqrt{2}x_1, \sqrt{2}x_2, 1)$$

• More expressive, as  $(x_1x_2)$  encodes

Stock+Market VS. Downtown+Market features

We can smartly compute the scalar product as

$$\Phi(\vec{x}) \cdot \Phi(\vec{z}) =$$

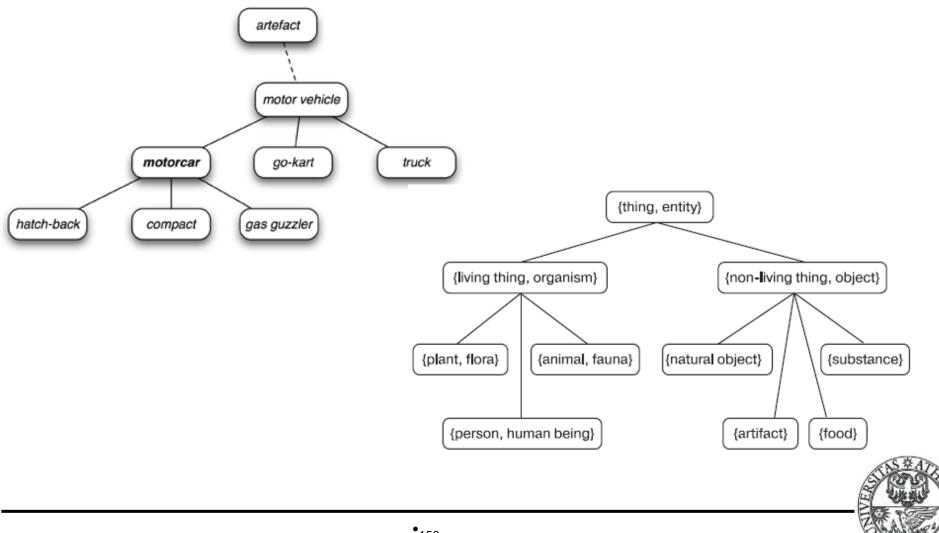
$$= (x_{1}^{2}, x_{2}^{2}, \sqrt{2}x_{1}x_{2}, \sqrt{2}x_{1}, \sqrt{2}x_{2}, 1) \cdot (z_{1}^{2}, z_{2}^{2}, \sqrt{2}z_{1}z_{2}, \sqrt{2}z_{1}, \sqrt{2}z_{2}, 1) =$$

$$= x_{1}^{2}z_{1}^{2} + x_{2}^{2}z_{2}^{2} + 2x_{1}x_{2}z_{1}z_{2} + 2x_{1}z_{1} + 2x_{2}z_{2} + 1 =$$

$$= (x_{1}z_{1} + x_{2}z_{2} + 1)^{2} = (\vec{x} \cdot \vec{z} + 1)^{2} = K_{Poly}(\vec{x}, \vec{z})$$



## **Sub-hierarchies in WordNet**



## Similarity based on WordNet

Inverted Path Length:

$$sim_{IPL}(c_1, c_2) = \frac{1}{(1 + d(c_1, c_2))^{\alpha}}$$

Wu & Palmer:

$$sim_{WUP}(c_1, c_2) = \frac{2 dep(lso(c_1, c_2))}{d(c_1, lso(c_1, c_2)) + d(c_2, lso(c_1, c_2)) + 2 dep(lso(c_1, c_2))}$$

Resnik:

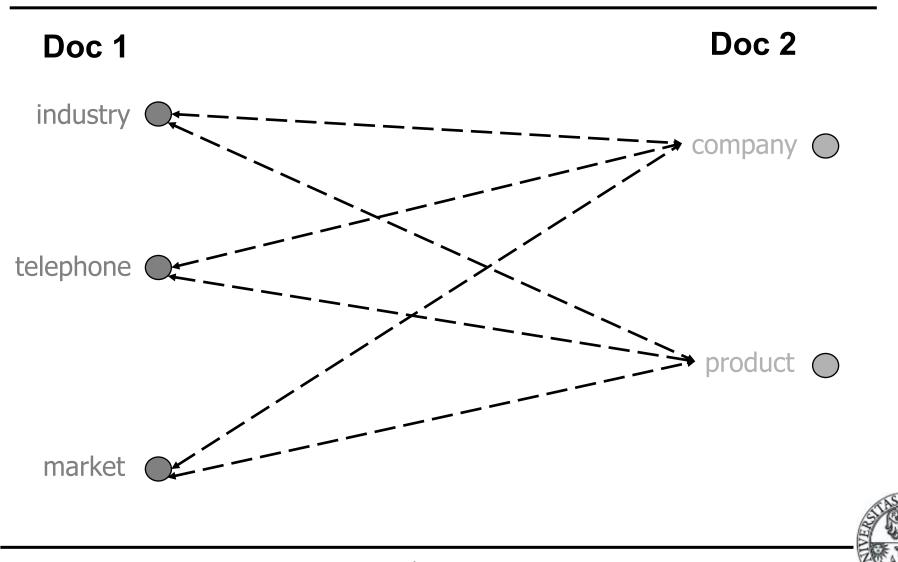
 $sim_{RES}(c_1, c_2) = -\log P(lso(c_1, c_2))$ 

Lin:

$$sim_{LIN}(c_1, c_2) = \frac{2 \log P(lso(c_1, c_2))}{\log P(c_1) + \log P(c_2)}$$



## **Document Similarity**



## **Lexical Semantic Kernels**

• The document similarity is the following SK function:

$$SK(d_1, d_2) = \sum_{w_1 \in d_1, w_2 \in d_2} S(w_1, w_2)$$

- where s is any similarity function between words, e.g.
   WordNet [Basili et al.,2005] similarity or LSA [Cristianini et al., 2002]
- Good results when training data is small



# **String Kernel**

- Given two strings, the number of matches between their substrings is evaluated
- E.g. Bank and Rank
  - B, a, n, k, Ba, Ban, Bank, Bk, an, ank, nk,...
  - R, a , n , k, Ra, Ran, Rank, Rk, an, ank, nk,...
- String kernel over sentences and texts
- Huge space but there are efficient algorithms



$$\phi("bank") = \vec{x} = (0,..,1,..,0,..,1,..,0,...,1,..,0,..,1,..,0,..,1,..,0)$$
  
bank ank bnk bk b

$$\phi("rank") = \vec{z} = (1,..,0,..,0,..,1,..,0,...,0,..,1,..,0,..,1,..,0,..,1)$$
  
rank ank rnk rk r

•  $\vec{x} \cdot \vec{z}$  counts the number of common substrings

$$\vec{x} \cdot \vec{z} = \phi("bank") \cdot \phi("rank") = k("bank","rank")$$



### **Formal Definition**

$$\begin{split} s &= s_1, .., s_{|s|}, \quad \vec{I} = (i_1, ..., i_{|u|}) \\ u &= s[\vec{I}] \\ \phi_u(s) &= \sum_{\vec{I}:u=s[\vec{I}]} \lambda^{l(\vec{I})}, \text{ where } l(\vec{I}) = i_{|u|} - i_1 + 1 \\ K(s,t) &= \sum_{u \in \Sigma^*} \phi_u(s) \cdot \phi_u(t) = \sum_{u \in \Sigma^*} \sum_{\vec{I}:u=s[\vec{I}]} \lambda^{l(\vec{I})} \sum_{\vec{J}:u=t[\vec{J}]} \lambda^{l(\vec{J})} = \\ &= \sum_{u \in \Sigma^*} \sum_{\vec{I}:u=s[\vec{I}]} \sum_{\vec{J}:u=t[\vec{J}]} \lambda^{l(\vec{I})+l(\vec{J})}, \text{ where } \Sigma^* = \bigcup_{n=0}^{\infty} \Sigma^n \end{split}$$

### Kernel between Bank and Rank

B, a, n, k, Ba, Ban, Bank, an, ank, nk, Bn, Bnk, Bk and ak are the substrings of Bank.

R, a, n, k, Ra, Ran, Rank, an, ank, nk, Rn, Rnk, Rk and ak are the substrings of *Rank*.



## An example of string kernel computation

- 
$$\phi_{a}(\text{Bank}) = \phi_{a}(\text{Rank}) = \lambda^{(i_{1}-i_{1}+1)} = \lambda^{(2-2+1)} = \lambda$$
,

- 
$$\phi_{n}(\text{Bank}) = \phi_{n}(\text{Rank}) = \lambda^{(i_{1}-i_{1}+1)} = \lambda^{(3-3+1)} = \lambda$$
,

- 
$$\phi_k(\text{Bank}) = \phi_k(\text{Rank}) = \lambda^{(i_1 - i_1 + 1)} = \lambda^{(4 - 4 + 1)} = \lambda$$
,

- 
$$\phi_{an}(Bank) = \phi_{an}(Rank) = \lambda^{(i_2-i_1+1)} = \lambda^{(3-2+1)} = \lambda^2$$
,

- 
$$\phi_{ank}(Bank) = \phi_{ank}(Rank) = \lambda^{(i_3-i_1+1)} = \lambda^{(4-2+1)} = \lambda^3$$
,

- 
$$\phi_{nk}(\text{Bank}) = \phi_{nk}(\text{Rank}) = \lambda^{(i_2 - i_1 + 1)} = \lambda^{(4 - 3 + 1)} = \lambda^2$$

-  $\phi_{ak}(Bank) = \phi_{ak}(Rank) = \lambda^{(i_2-i_1+1)} = \lambda^{(4-2+1)} = \lambda^3$ 

$$\begin{split} &K(\text{Bank},\text{Rank}) = (\lambda,\lambda,\lambda,\lambda^2,\lambda^3,\lambda^2,\lambda^3) \cdot (\lambda,\lambda,\lambda,\lambda^2,\lambda^3,\lambda^2,\lambda^3) \\ &= 3\lambda^2 + 2\lambda^4 + 2\lambda^6 \end{split}$$



## **Efficient Evaluation: Intuition**

- Dynamic Programming technique over:
  - The size of the two input strings, *m*, *n* and
  - The size of their common substrings, p
- Evaluate the spectrum string kernels
  - Substrings of size p
- Sum the contribution of the different p spectra



#### **Efficient Evaluation**

Given two sequences  $s_1a$  and  $s_2b$ , we define:

$$D_p(|s_1|, |s_2|) = \sum_{i=1}^{|s_1|} \sum_{r=1}^{|s_2|} \lambda^{|s_1|-i+|s_2|-r} \times SK_{p-1}(s_1[1:i], s_2[1:r]),$$

 $s_1[1:i]$  and  $s_2[1:r]$  are their subsequences from 1 to i and 1 to r.

$$SK_p(s_1a, s_2b) = \begin{cases} \lambda^2 \times D_p(|s_1|, |s_2|) \text{ if } a = b; \\ 0 & otherwise. \end{cases}$$

 $D_p$  satisfies the recursive relation:

$$D_p(k,l) = SK_{p-1}(s_1[1:k], s_2[1:l]) + \lambda D_p(k,l-1) + \lambda D_p(k-1,l) - \lambda^2 D_p(k-1,l-1)$$

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# **Evaluating DP2**

- Evaluate the weight of the string of size p in case a character will be matched
- This is done by multiplying the double summation by the number of substrings of size p-1

$$D_p(|s_1|, |s_2|) = \sum_{i=1}^{|s_1|} \sum_{r=1}^{|s_2|} \lambda^{|s_1|-i+|s_2|-r} \times SK_{p-1}(s_1[1:i], s_2[1:r])$$



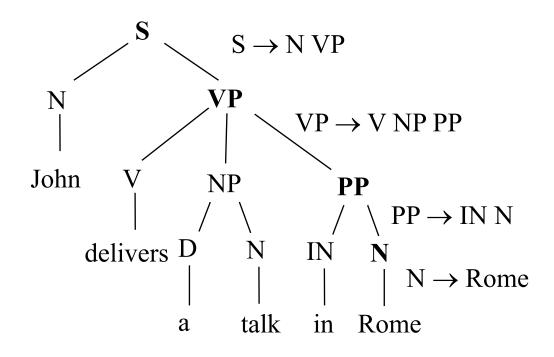
## **Tree kernels**

- Syntactic Tree Kernel, Partial Tree kernel (PTK),
   Semantic Syntactic Tree Kernel, Smoothed PTK
- Efficient computation



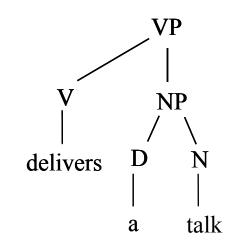
### **Example of a parse tree**

"John delivers a talk in Rome"



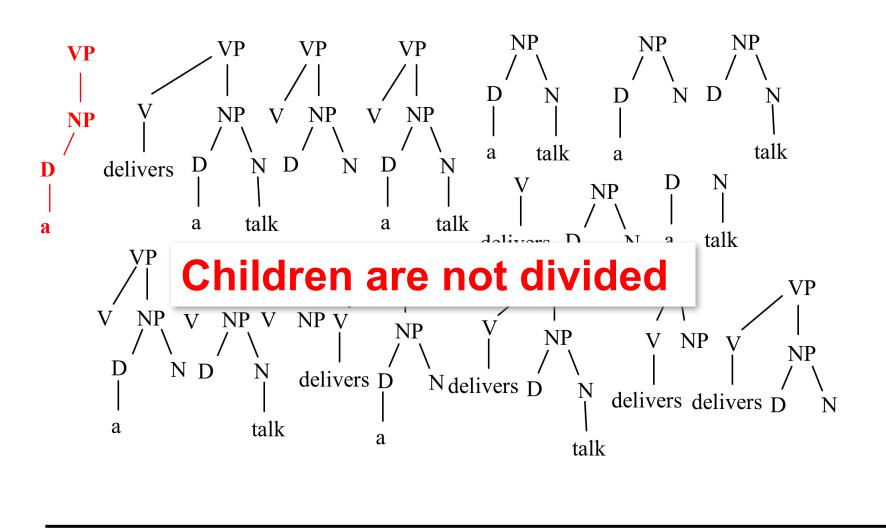


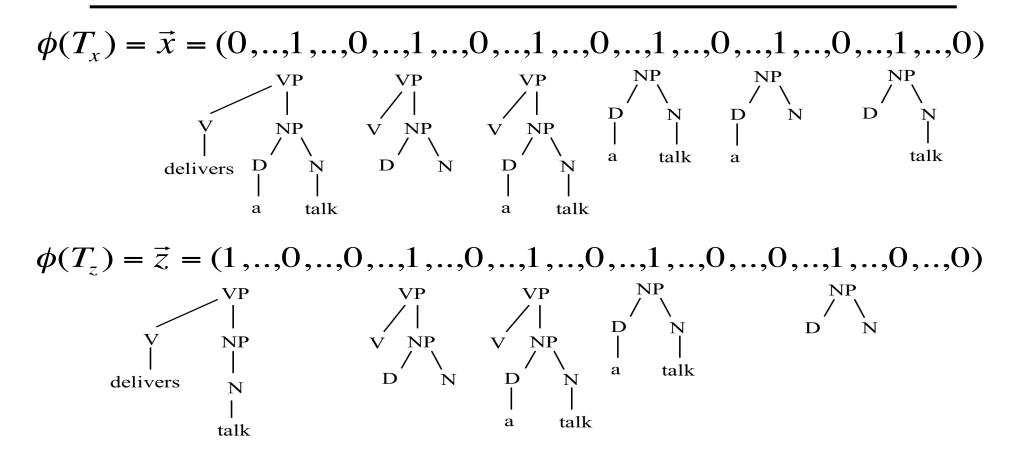
#### The Syntactic Tree Kernel (STK) [Collins and Duffy, 2002]





## The overall fragment set





•  $\vec{\chi} \cdot \vec{z}$  counts the number of common substructures



#### Efficient evaluation of the scalar product

$$\vec{x} \cdot \vec{z} = \phi(T_x) \cdot \phi(T_z) = K(T_x, T_z) =$$
$$= \sum_{n_x \in T_x} \sum_{n_z \in T_z} \Delta(n_x, n_z)$$



#### Efficient evaluation of the scalar product

$$\vec{x} \cdot \vec{z} = \phi(T_x) \cdot \phi(T_z) = K(T_x, T_z) =$$
$$= \sum_{n_x \in T_x} \sum_{n_z \in T_z} \Delta(n_x, n_z)$$

• [Collins and Duffy, ACL 2002] evaluate  $\Delta$  in O(n<sup>2</sup>):

 $\Delta(n_x, n_z) = 0, \text{ if the productions are different else}$   $\Delta(n_x, n_z) = 1, \text{ if pre-terminals else}$  $\Delta(n_x, n_z) = \prod_{j=1}^{nc(n_x)} (1 + \Delta(ch(n_x, j), ch(n_z, j)))$ 



## **Other Adjustments**

Decay factor

$$\Delta(n_x, n_z) = \lambda, \text{ if pre-terminals else}$$
  
$$\Delta(n_x, n_z) = \lambda \prod_{j=1}^{nc(n_x)} (1 + \Delta(ch(n_x, j), ch(n_z, j)))$$

Normalization

$$K'(T_x, T_z) = \frac{K(T_x, T_z)}{\sqrt{K(T_x, T_x) \times K(T_z, T_z)}}$$

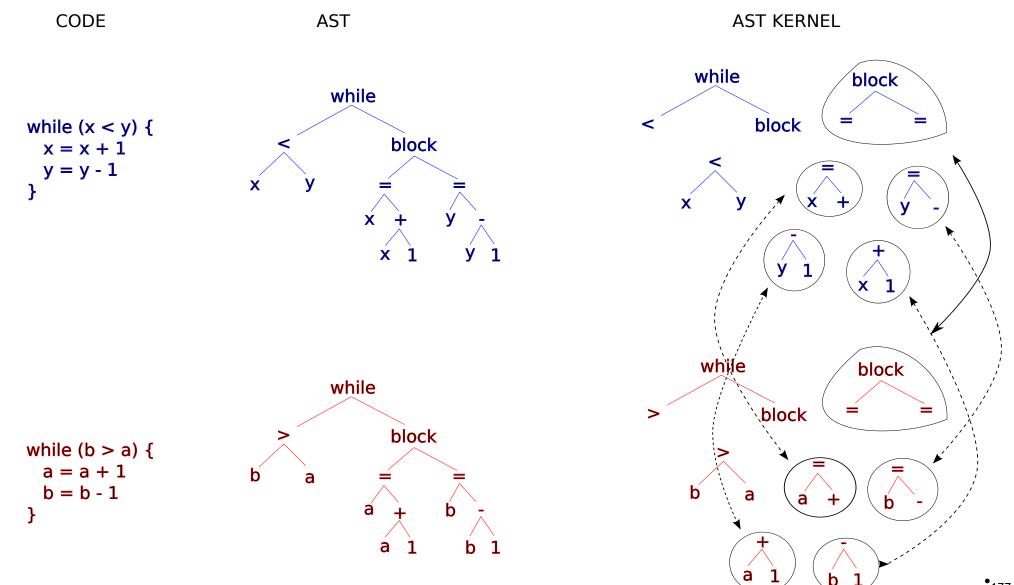


## Observations

- We can order the production rules used in T<sub>x</sub> and T<sub>z</sub>, at loading time
- At learning time we can evaluate NP in  $|T_x|+|T_z|$  running time [Moschitti, EACL 2006]
- If  $T_x$  and  $T_z$  are generated by only one production rule  $\Rightarrow$ O( $|T_x| \times |T_z|$ )...*Very Unlikely!!!!*

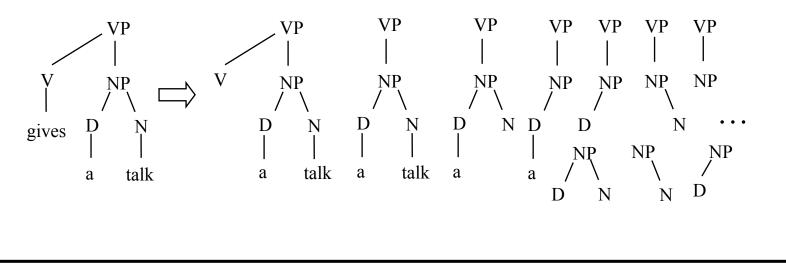


#### Trees can also be program derivation trees



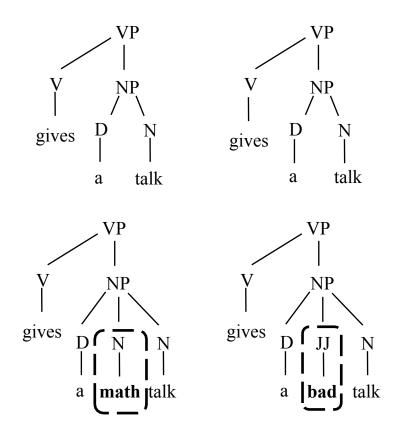
## Labeled Ordered Tree Kernel

- STK satisfies the constraint "remove 0 or all children at a time".
- If we relax such constraint we get more general substructures [Kashima and Koyanagi, 2002]





# **Weighting Problems**

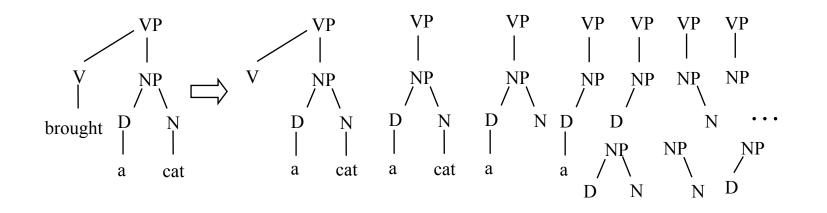


- Both matched pairs give the same contribution
- Gap based weighting is needed
- A novel efficient evaluation has to be defined



#### Partial Tree Kernel (PTK) [Moschitti, ECML 2006]

STK + String Kernel with weighted gaps on nodes' children





## **Partial Tree Kernel - Definition**

- if the node labels of  $n_1$  and  $n_2$  are different then  $\Delta(n_1, n_2) = 0;$ 

- else  $\Delta(n_1, n_2) = 1 + \sum_{\vec{J}_1, \vec{J}_2, l(\vec{J}_1) = l(\vec{J}_2)} \prod_{i=1}^{l(\vec{J}_1)} \Delta(c_{n_1}[\vec{J}_{1i}], c_{n_2}[\vec{J}_{2i}])$
- By adding two decay factors we obtain:

$$\mu \left( \lambda^2 + \sum_{\vec{J}_1, \vec{J}_2, l(\vec{J}_1) = l(\vec{J}_2)} \lambda^{d(\vec{J}_1) + d(\vec{J}_2)} \prod_{i=1}^{l(\vec{J}_1)} \Delta(c_{n_1}[\vec{J}_{1i}], c_{n_2}[\vec{J}_{2i}]) \right)$$



# Efficient Evaluation (1)

- In [Taylor and Cristianini, 2004 book], sequence kernels with weighted gaps are factorized with respect to different subsequence sizes
- We treat children as sequences and apply the same theory

$$\Delta(n_1, n_2) = \mu \left( \lambda^2 + \sum_{p=1}^{lm} \Delta_p(c_{n_1}, c_{n_2}) \right)$$

Given the two child sequences  $s_1a = c_{n_1}$  and  $s_2b = c_{n_2}$ (*a* and *b* are the last children),  $\Delta_p(s_1a, s_2b) =$ 

$$\Delta(a,b) \times \sum_{i=1}^{|s_1|} \sum_{r=1}^{|s_2|} \lambda^{|s_1|-i+|s_2|-r} \times \Delta_{p-1}(s_1[1:i], s_2[1:r])$$

# Efficient Evaluation (2)

$$\Delta_p(s_1a, s_2b) = \begin{cases} \Delta(a, b)D_p(|s_1|, |s_2|) \text{ if } a = b; \\ 0 & otherwise. \end{cases}$$

Note that  $D_p$  satisfies the recursive relation:

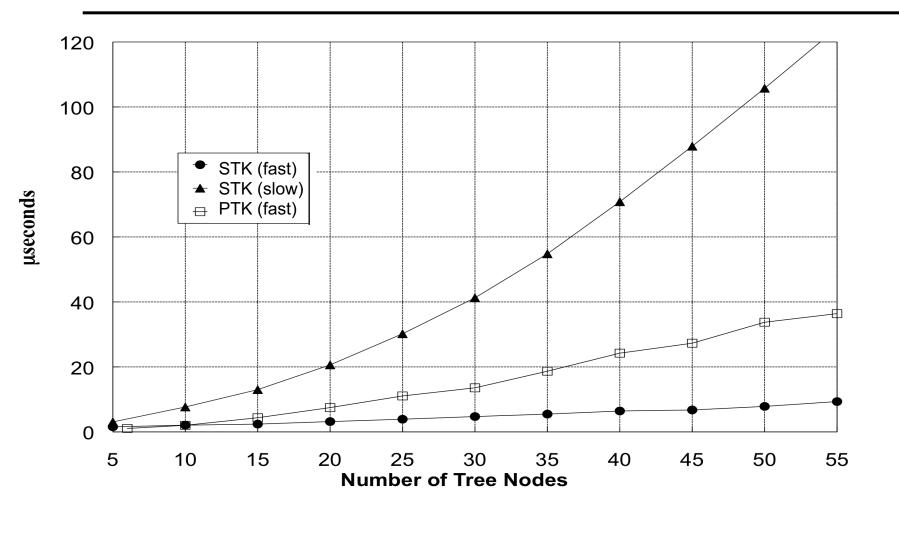
$$D_p(k,l) = \Delta_{p-1}(s_1[1:k], s_2[1:l]) + \lambda D_p(k,l-1) + \lambda D_p(k-1,l) + \lambda^2 D_p(k-1,l-1).$$

• The complexity of finding the subsequences is  $O(p|s_1||s_2|)$ 

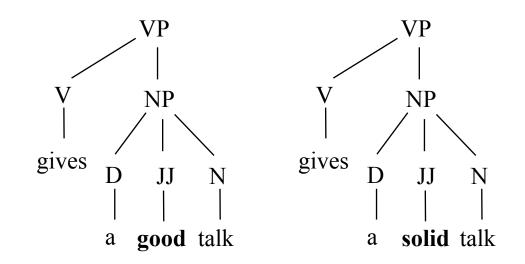
• Therefore the overall complexity is  $O(p\rho^2|N_{T_1}||N_{T_2}|)$ where  $\rho$  is the maximum branching factor ( $p = \rho$ )



# **Running Time of Tree Kernel Functions**



### Syntactic/Semantic Tree Kernels (SSTK) [Bloehdorn & Moschitti, ECIR 2007 & CIKM 2007]



Similarity between the fragment leaves

Tree kernel + Lexical Similarity Kernel



**Definition 4 (Tree Fragment Similarity Kernel).** For two tree fragments  $f_1, f_2 \in \mathcal{F}$ , we define the Tree Fragment Similarity Kernel  $as^6$ :

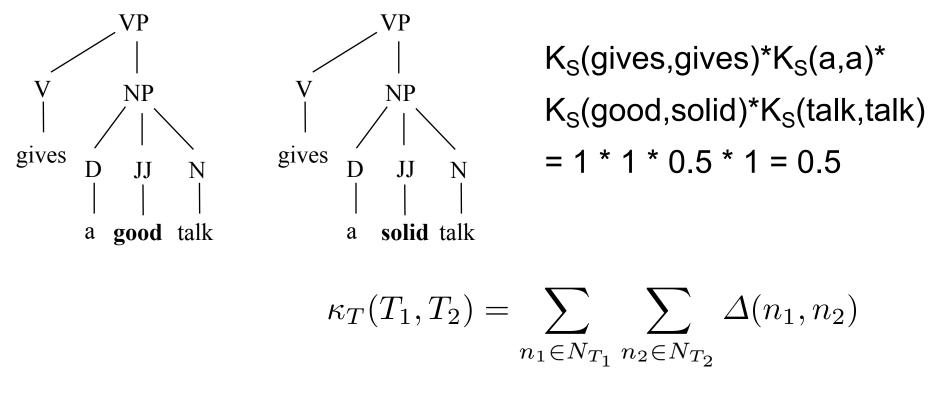
$$\kappa_{\mathcal{F}}(f_1, f_2) = comp(f_1, f_2) \prod_{t=1}^{nt(f_1)} \kappa_S(f_1(t), f_2(t))$$

$$\kappa_T(T_1, T_2) = \sum_{n_1 \in N_{T_1}} \sum_{n_2 \in N_{T_2}} \Delta(n_1, n_2)$$

where 
$$\Delta(n_1, n_2) = \sum_{i=1}^{|\mathcal{F}|} \sum_{j=1}^{|\mathcal{F}|} I_i(n_1) I_j(n_2) \kappa_{\mathcal{F}}(f_i, f_j).$$



# **Example of an SSTK evaluation**



where 
$$\Delta(n_1, n_2) = \sum_{i=1}^{|\mathcal{F}|} \sum_{j=1}^{|\mathcal{F}|} I_i(n_1) I_j(n_2) \kappa_{\mathcal{F}}(f_i, f_j).$$



# **Delta Evaluation is very simple**

- 0. if  $n_1$  and  $n_2$  are pre-terminals and  $label(n_1) = label(n_2)$  then  $\Delta(n_1, n_2) = \lambda \kappa_{\mathcal{S}}(ch_{n_1}^1, ch_{n_2}^1)$ ,
- 1. if the productions at  $n_1$  and  $n_2$  are different then  $\Delta(n_1, n_2) = 0$ ;
- 2.  $\Delta(n_1, n_2) = \lambda$ , 3.  $\Delta(n_1, n_2) = \lambda \prod_{j=1}^{nc(n_1)} (1 + \Delta(ch_{n_1}^j, ch_{n_2}^j)).$



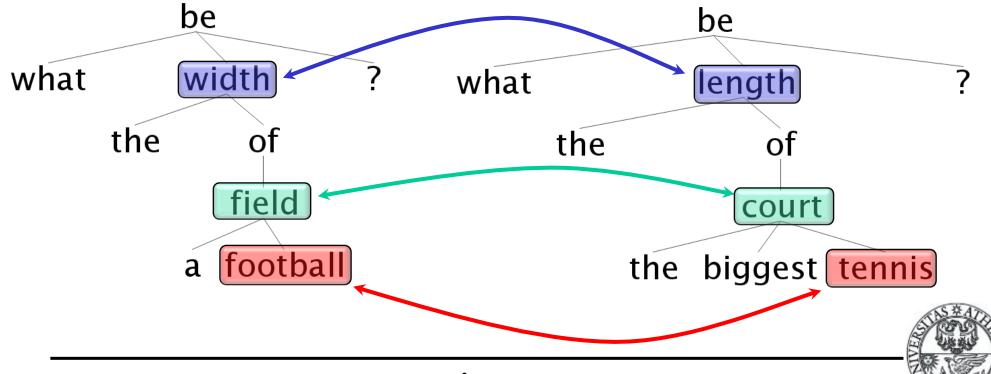
### **Smoothed Partial Tree Kernels** [Moschitti, EACL 2009; Croce et al., 2011]

- Same idea of Syntactic Semantic Tree Kernel but the similarity is extended to any node of the tree
- The tree fragments are those generated by PTK
- Basically it extends PTK with similarities

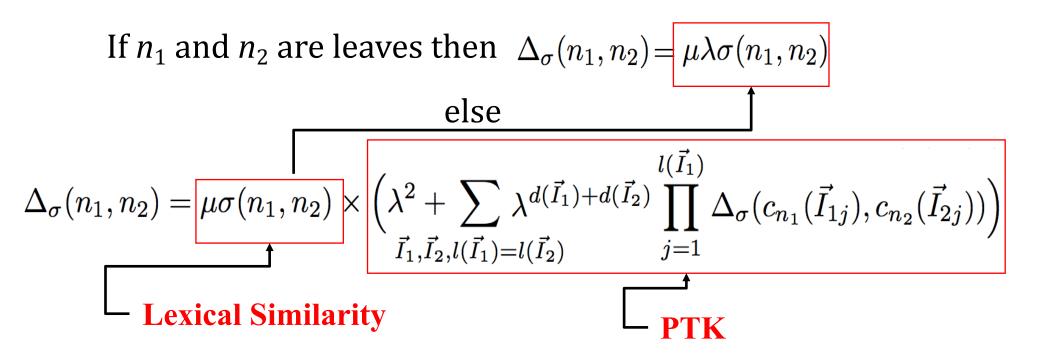


# **Examples of Dependency Trees**

- What is the width of a football field?
- What is the length of the biggest tennis court?

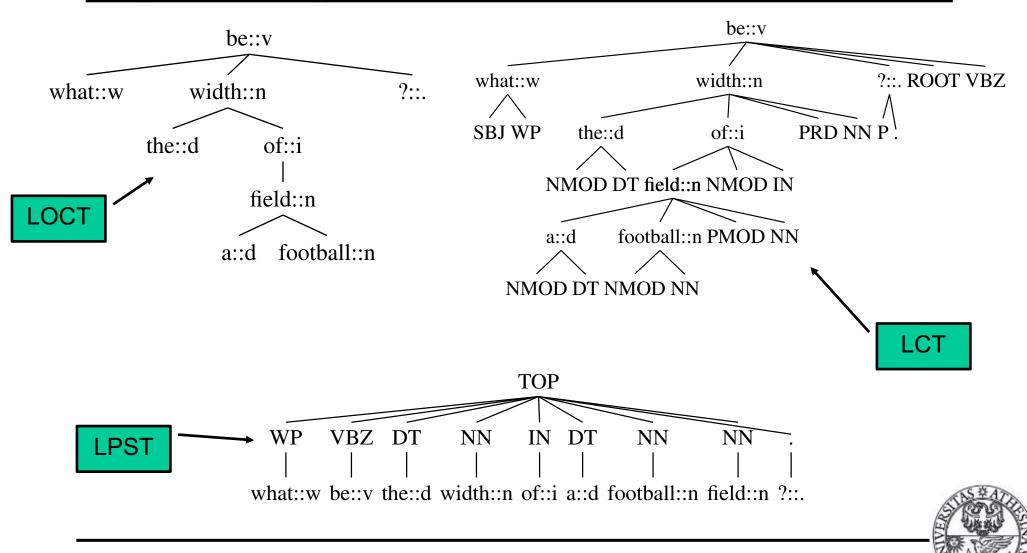


# **Equation of SPTK**

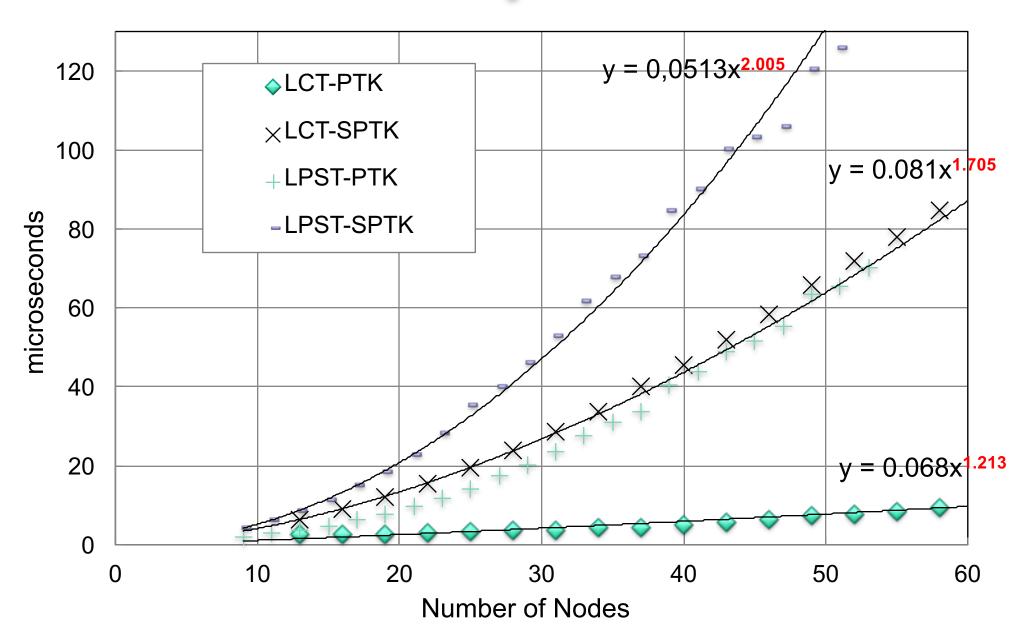




# Different versions of Computational Dependency Trees for PTK/SPTK



## **Tree Kernel Efficiency**

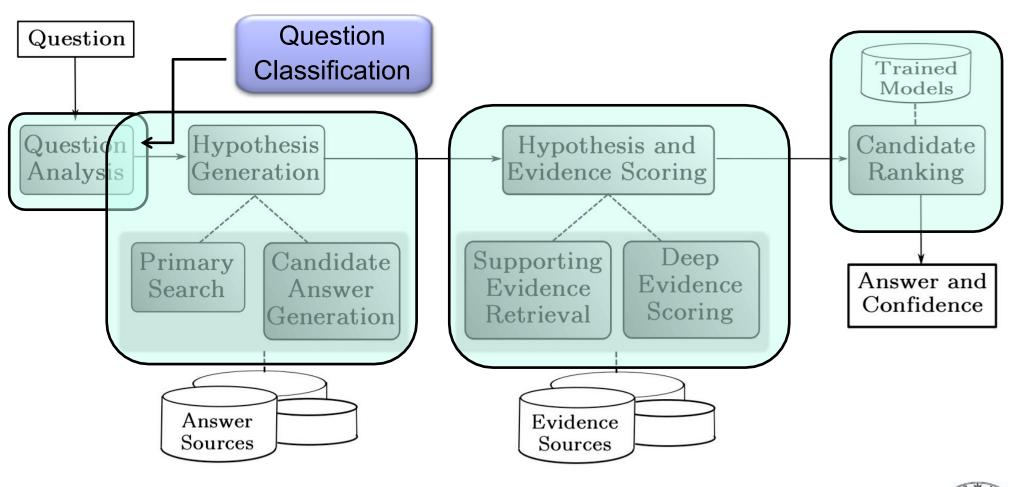


# **Outline:** Part I – Classification with Kernels

Classification with Kernels (15 min)

- Question Classification (QC) using constituency, dependency and semantic structures
- Question Classification (QC) in Jeopardy!
- Relation Extraction with kernels
- Kernel-Based Coreference Resolution

# **IBM Watson (simplified) Pipeline**





# **Question Classification**

- **Definition**: What does HTML stand for?
- Description: What's the final line in the Edgar Allan Poe poem "The Raven"?
- **Entity**: What foods can cause allergic reaction in people?
- **Human**: Who won the Nobel Peace Prize in 1992?
- **Location**: Where is the Statue of Liberty?
- Manner: How did Bob Marley die?
- Numeric: When was Martin Luther King Jr. born?
- Organization: What company makes Bentley cars?



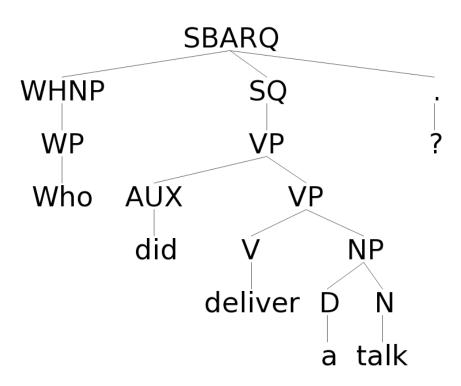
# **Question Classifier based on Tree Kernels**

- Question dataset (http://l2r.cs.uiuc.edu/~cogcomp/Data/QA/QC/)
   [Lin and Roth, 2005])
  - Distributed on 6 categories: Abbreviations, Descriptions, Entity, Human, Location, and Numeric.
- Fixed split 5500 training and 500 test questions
- Using the whole question parse trees
  - Constituent parsing
  - Example

### "Who did deliver a talk?"

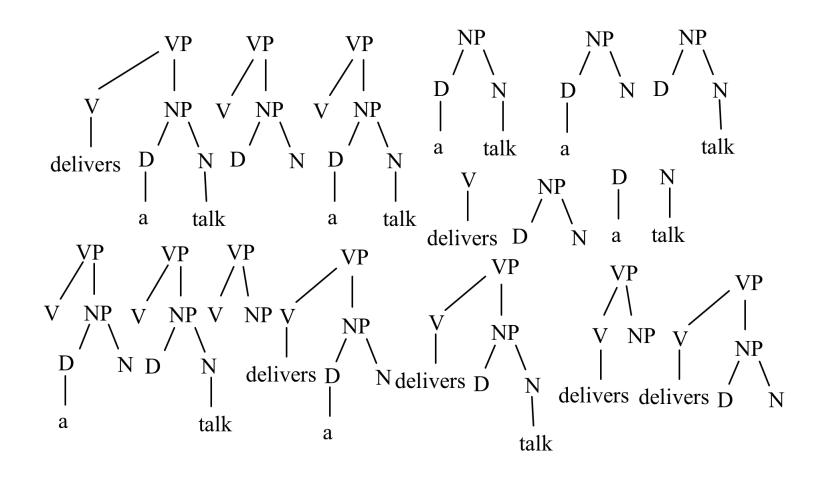


# Syntactic Parse Trees (PT)

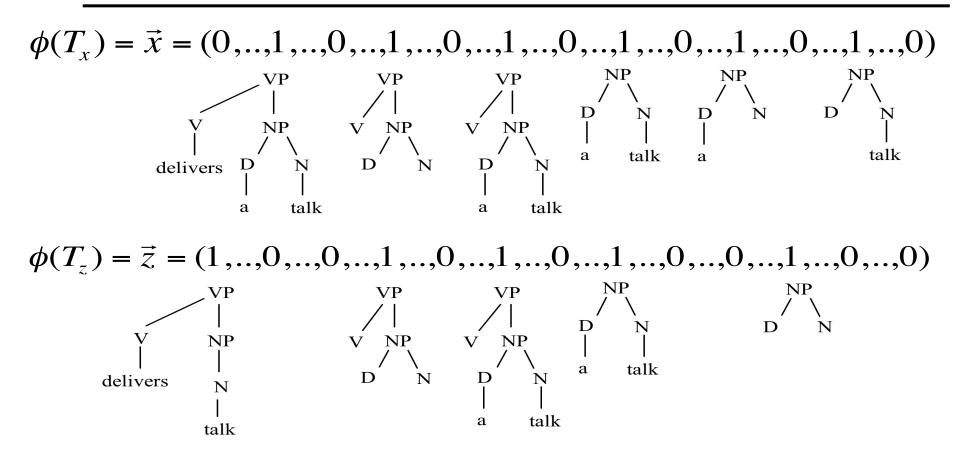




## Some fragments from the VP subtree







•  $\vec{\chi} \cdot \vec{z}$  counts the number of common substructures



## Question Classification with SSTK [Blohedorn&Moschitti, CIKM2007]

#### **Syntactic Tree Kernel**



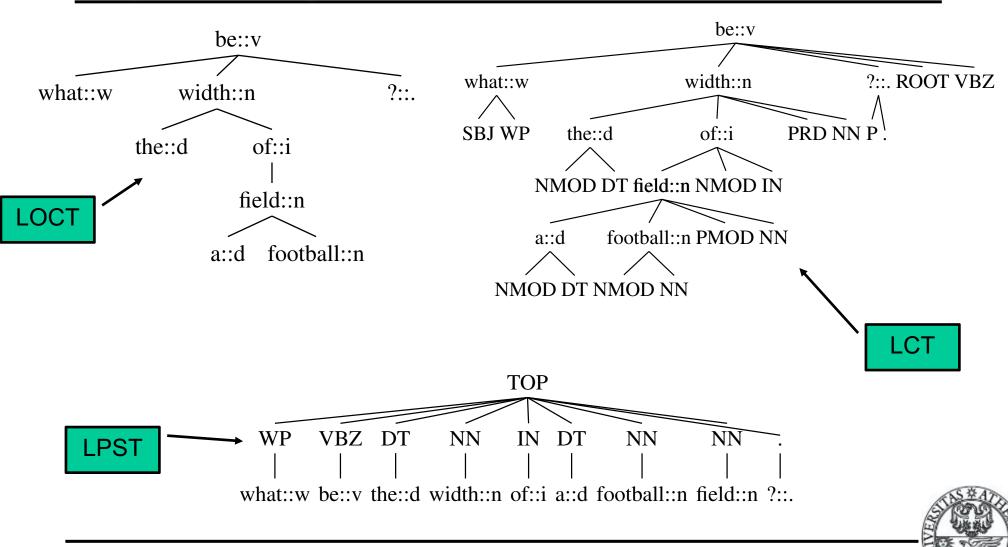
13)								
		Accuracy						
	$\lambda$ parameter	0.4	0.05	0.01	0.005	0.001		
	linear (bow)	0.905						
	string matching	0.890	0.910	0.914	0.914	0.912		
	full	0.904	0.924	0.918	0.922	0.920		
	full-ic	0.908	0.922	0.916	0.918	0.918		
	path-1	0.906	0.918	0.912	0.918	0.916		
	$\mathbf{path-2}$	0.896	0.914	0.914	0.916	0.916		
	lin	0.908	0.924	0.918	0.922	0.922		
	wup	0.908	0.926	0.918	0.922	0.922		

Syntactic Tree Kernel

with similarities (SSTK)



# Same Task with PTK, SPTK and Dependency Trees



### State-of-the-art Results [Croce et al., EMNLP 2011]

	STK	РТК	SPTK(LSA)
СТ	91.20%	90.80%	91.00%
LOCT	-	89.20%	93.20%
LCT	-	90.80%	94.80%
LPST	-	89.40%	89.60%
BOW		88.80%	



# Classification, Ranking, Regression and Multiclassification



## The Ranking SVM [Herbrich et al. 1999, 2000; Joachims et al. 2002]

- The aim is to classify instance pairs as correctly ranked or incorrectly ranked
  - This turns an ordinal regression problem back into a binary classification problem
- We want a ranking function f such that

 $\boldsymbol{x}_i > \boldsymbol{x}_j \text{ iff } f(\boldsymbol{x}_i) > f(\boldsymbol{x}_j)$ 

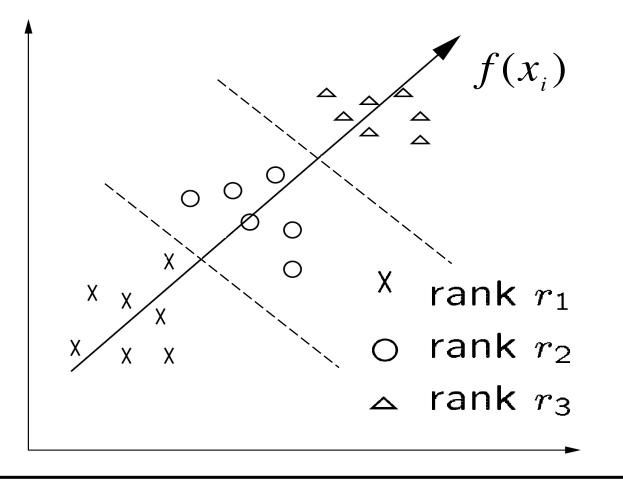
- or at least one that tries to do this with minimal error
- Suppose that f is a linear function

$$f(\boldsymbol{x}_i) = \mathbf{w} \bullet \boldsymbol{x}_i$$



# The Ranking SVM

Ranking Model:  $f(\mathbf{x}_i)$ 





# The Ranking SVM

Then (combining the two equations on the last slide):

$$\boldsymbol{x}_i > \boldsymbol{x}_j \text{ iff } \boldsymbol{w} \cdot \boldsymbol{x}_i - \boldsymbol{w} \cdot \boldsymbol{x}_j > 0$$

$$\boldsymbol{x}_i > \boldsymbol{x}_j \text{ iff } \boldsymbol{w} \cdot (\boldsymbol{x}_i - \boldsymbol{x}_j) > 0$$

Let us then create a new instance space from such pairs:  $z_k = x_i - x_k$ 

$$y_k = +1, -1 \text{ as } x_i \ge < x_k$$



# **Support Vector Ranking**

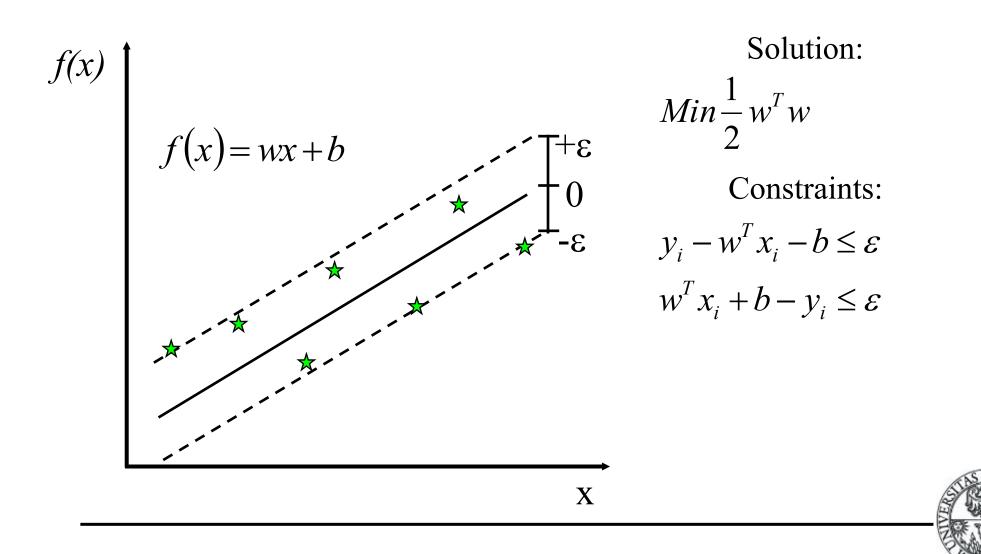
$$\begin{cases} \min \quad \frac{1}{2} ||\vec{w}|| + C \sum_{i=1}^{m} \xi_i^2 \\ y_k(\vec{w} \cdot (\vec{x_i} - \vec{x_j}) + b) \ge 1 - \xi_k, \quad \forall i, j = 1, ..., m \\ \xi_k \ge 0, \quad k = 1, ..., m^2 \end{cases}$$

 $y_k = 1$  if  $rank(\vec{x_i}) > rank(\vec{x_j})$ ,-1 otherwise, where  $k = i \times m + j$ 

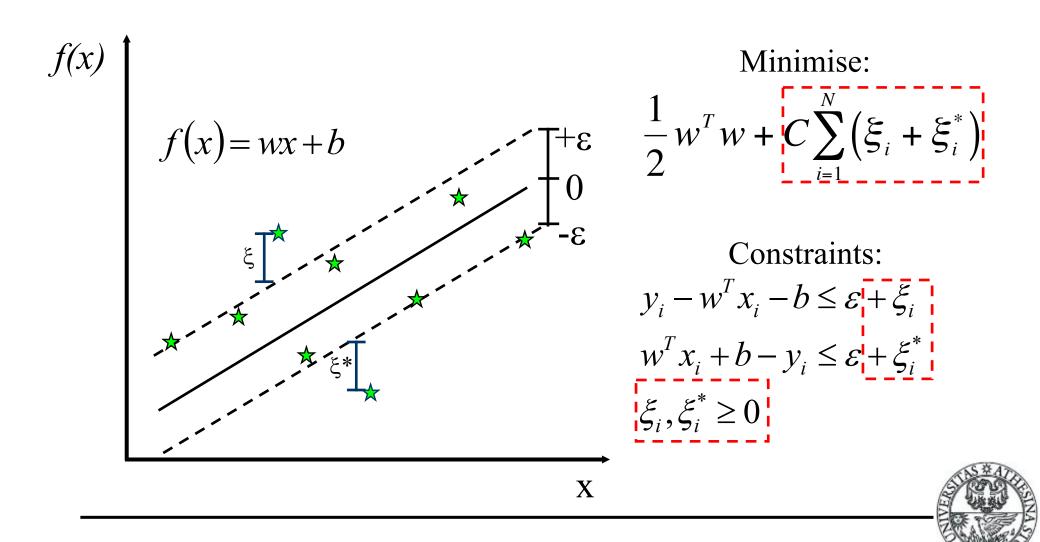
### Given two examples we build one example $(x_i, x_j)$



# Support Vector Regression (SVR)



# Support Vector Regression (SVR)



# **Support Vector Regression**

$$\min_{\mathbf{w},b,\xi,\xi^*} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^n (\xi_i + \xi_i^*)$$
s.t.  $y_i - \mathbf{w}^\top \mathbf{x}_i - b \le \epsilon + \xi_i, \ \xi_i \ge 0 \quad \forall 1 \le i \le n;$   
 $\mathbf{w}^\top \mathbf{x}_i + b - y_i \le \epsilon + \xi_i^*, \ \xi_i^* \ge 0 \quad \forall 1 \le i \le n.$ 

- $y_i$  is not -1 or 1 anymore, now it is a value
- $\varepsilon$  is the tollerance of our function value



# **From Binary to Multiclass classifiers**

- Three different approaches:
- ONE-vs-ALL (OVA)
  - Given the example sets, {E1, E2, E3, …} for the categories: {C1, C2, C3,…} the binary classifiers: {b1, b2, b3,…} are built.
  - For b1, E1 is the set of positives and E2∪E3 ∪... is the set of negatives, and so on
  - For testing: given a classification instance x, the category is the one associated with the maximum margin among all binary classifiers



# **From Binary to Multiclass classifiers**

### ALL-vs-ALL (AVA)

- Given the examples: {E1, E2, E3, …} for the categories {C1, C2, C3,…}
  - build the binary classifiers:

 $\label{eq:b1_2,b1_3,...,b1_n,b2_3,b2_4,...,b2_n,...,bn-1_n} \\$ 

- by learning on E1 (positives) and E2 (negatives), on E1 (positives) and E3 (negatives) and so on...
- For testing: given an example x,
  - all the votes of all classifiers are collected
  - where b<sub>E1E2</sub> = 1 means a vote for C1 and b<sub>E1E2</sub> = -1 is a vote for C2
- Select the category that gets more votes



# Natural Language Processing and Information Retrieval

## **Structured Output**

### Alessandro Moschitti

Department of information and communication technology University of Trento Email: moschitti@dit.unitn.it



# **Simple Structured Output**

- We have seen methods for: binary Classifier or multiclassifier single label
- Multiclass-Multilabel is a structured output, i.e. a label subset is output



# **From Binary to Multiclass classifiers**

- Three different approaches:
- ONE-vs-ALL (OVA)
  - Given the example sets, {E1, E2, E3, …} for the categories: {C1, C2, C3,…} the binary classifiers: {b1, b2, b3,…} are built.
  - For b1, E1 is the set of positives and E2∪E3 ∪... is the set of negatives, and so on
  - For testing: given a classification instance x, the category is the one associated with the maximum margin among all binary classifiers



### **From Binary to Multiclass classifiers**

### ALL-vs-ALL (AVA)

- Given the examples: {E1, E2, E3, …} for the categories {C1, C2, C3,…}
  - build the binary classifiers:

 $b1_2, b1_3, ..., b1_n, b2_3, b2_4, ..., b2_n, ..., bn-1_n$ 

- by learning on E1 (positives) and E2 (negatives), on E1 (positives) and E3 (negatives) and so on...
- For testing: given an example x,
  - all the votes of all classifiers are collected
  - where b<sub>E1E2</sub> = 1 means a vote for C1 and b<sub>E1E2</sub> = -1 is a vote for C2
- Select the category that gets more votes



### **From Binary to Multiclass classifiers**

### Error Correcting Output Codes (ECOC)

- The training set is partitioned according to binary sequences (codes) associated with category sets.
  - For example, 10101 indicates that the set of examples of C1,C3 and C5 are used to train the  $C_{10101}$  classifier.
  - The data of the other categories, i.e. C2 and C4 will be negative examples
- In testing: the code-classifiers are used to decode one the original class, e.g.

 $C_{10101} = 1$  and  $C_{11010} = 1$  indicates that the instance belongs to C1 That is, the only one consistent with the codes



# **Designing Global Classifiers**

- Each class has a parameter vector  $(w_k, b_k)$
- x is assigned to class k iff

$$w_k^\top x + b_k \ge \max_j w_j^\top x + b_j$$

- For simplicity set b<sub>k</sub>=0
   (add a dimension and include it in w<sub>k</sub>)
- The goal (given separable data) is to choose  $w_k$  s.t.

$$\forall (x^i, y^i), \quad w_{y^i}^\top x^i \geq \max_j w_j^\top x^i$$



### Multi-class SVM

### Primal problem: QP

$$\min_{w_1,...,w_K} \quad \frac{1}{2} \| (w_1,...,w_K) \|^2 + C \sum_{ik} \xi_{ik}$$
  
s.t.  $\forall (i,k), \quad w_{y^i}^\top x^i - w_k^\top x^i \ge \mathbf{1} \{ k \neq y^i \} - \xi_{ik}$ 



# **Structured Output Model**

Main idea: define scoring function which
 decomposes as sum of features scores k on
 "parts" p:

$$score(\mathbf{x}, \mathbf{y}, \mathbf{w}) = \mathbf{w}^{\top} \Phi(\mathbf{x}, \mathbf{y}) = \sum_{k, p} w_k^{\top} \phi_k(\mathbf{x}_p, \mathbf{y}_p)$$

Label examples by looking for max score:

$$prediction(\mathbf{x}, \mathbf{w}) = \arg \max score(\mathbf{x}, \mathbf{y}, \mathbf{w})$$
$$\mathbf{y} \in \mathcal{Y}(\mathbf{x})$$
Space of feasible outputs



### **Structured Perceptron**

Training set  $(x_i, y_i)$  for  $i = 1 \dots n$ **Inputs:** Initialization:  $\mathbf{W} = 0$  $F(x) = \operatorname{argmax}_{u \in \mathbf{GEN}(x)} \mathbf{\Phi}(x, y) \cdot \mathbf{W}$ **Define:** For t = 1 ... T, i = 1 ... n**Algorithm:**  $z_i = F(x_i)$ If  $(z_i \neq y_i)$   $\mathbf{W} = \mathbf{W} + \mathbf{\Phi}(x_i, y_i) - \mathbf{\Phi}(x_i, z_i)$ Parameters W **Output:** 



# (Averaged) Perceptron

For each datapoint  $\mathbf{x}^i$ 

Predict:
$$\hat{\mathbf{y}}_i = \arg \max_{\mathbf{y} \in \mathcal{Y}} \mathbf{w}_t^\top \Phi(\mathbf{x}^i, \mathbf{y})$$
Update: $\mathbf{w}_{t+1} = \mathbf{w}_t + \alpha \underbrace{\left(\Phi(\mathbf{x}, \mathbf{y}^i) - \Phi(\mathbf{x}^i, \hat{\mathbf{y}}_i)\right)}_{\text{update if } \hat{\mathbf{y}}_i \neq \mathbf{y}^i}$ 

### Averaged perceptron:

$$\bar{\mathbf{w}} = \frac{1}{T} \sum_{t=1}^{T} \mathbf{w}_t$$

### **Example: multiclass setting**

**Predict:** 

Predict: 
$$\hat{y}_i = \arg \max_{y} w_y^{\top} x^i$$
  
Update: if  $\hat{y}_i \neq y^i$  then  
 $w_{y^i,t+1} = w_{y^i,t} + \alpha x^i$   
 $w_{\hat{y}_i,t+1} = w_{\hat{y}_i,t} - \alpha x^i$ 

Feature encoding:  

$$\Phi(\mathbf{x}^{i}, y = 1)^{\top} = [\mathbf{x}^{i^{\top}} 0 \dots 0]$$

$$\Phi(\mathbf{x}^{i}, y = 2)^{\top} = [0 \mathbf{x}^{i^{\top}} \dots 0]$$

$$\vdots$$

$$\Phi(\mathbf{x}^{i}, y = K)^{\top} = [0 0 \dots \mathbf{x}^{i^{\top}}]$$

$$\mathbf{w}^{\top} = [w_{1}^{\top} w_{2}^{\top} \dots w_{K}^{\top}]$$

 $\widehat{\mathbf{y}}_i = rg\max_{\mathbf{y} \in \mathcal{Y}} \mathbf{w}_t^{ op} \Phi(\mathbf{x}^i, \mathbf{y})$ 

Update: 
$$\mathbf{w}_{t+1} = \mathbf{w}_t + \alpha \underbrace{\left(\Phi(\mathbf{x}, \mathbf{y}^i) - \Phi(\mathbf{x}^i, \widehat{\mathbf{y}}_i)\right)}_{\text{update if } \widehat{\mathbf{y}}_i \neq \mathbf{y}^i}$$

### **Output of Ranked Example List**



# **Support Vector Ranking**

$$\begin{cases} \min \quad \frac{1}{2} ||\vec{w}|| + C \sum_{i=1}^{m} \xi_i^2 \\ y_k(\vec{w} \cdot (\vec{x_i} - \vec{x_j}) + b) \ge 1 - \xi_k, \quad \forall i, j = 1, ..., m \\ \xi_k \ge 0, \quad k = 1, ..., m^2 \end{cases}$$

 $y_k = 1$  if  $rank(\vec{x_i}) > rank(\vec{x_j})$ , 0 otherwise, where  $k = i \times m + j$ 

Given two examples we build one example  $(x_i, x_j)$ 



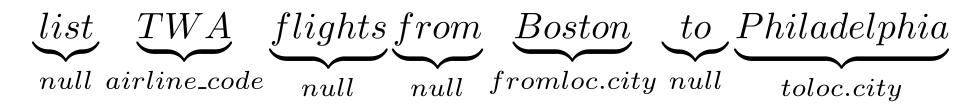
# Concept Segmentation and Classification task

- Given a transcription, i.e. a sequence of words, chunk and label subsequences with concepts
- Air Travel Information System (ATIS)
  - Dialog systems answering user questions
  - Conceptually annotated dataset
  - Frames



# An example of concept annotation in ATIS

# User request: *list TWA flights from Boston to Philadelphia*



- The concepts are used to build rules for the dialog manager (e.g. actions for using the DB)
  - from location
  - to location
  - airline code

list flights from boston to Philadelphia FRAME: FLIGHT FROMLOC.CITY = boston TOLOC.CITY = Philadelphia



### **Our Approach** (Dinarelli, Moschitti, Riccardi, SLT 2008)

- Use of Finite State Transducer to generate word sequences and concepts
- Probability of each annotation
- $\Rightarrow$  *m* best hypothesis can be generated
- Idea: use a discriminative model to choose the best one
  - Re-ranking and selecting the top one



### **Experiments**

### Luna projects' Corpus Wizard of OZ

Corpus LUNA	Training set		Test set	
	words	concepts	words	concepts
Dialogs	183		67	
Turns	1,019		373	
Tokens	8,512	2,887	2,888	984
Vocabulary	1,172	34	-	-
OOV rate	_	-	3.2%	0.1%

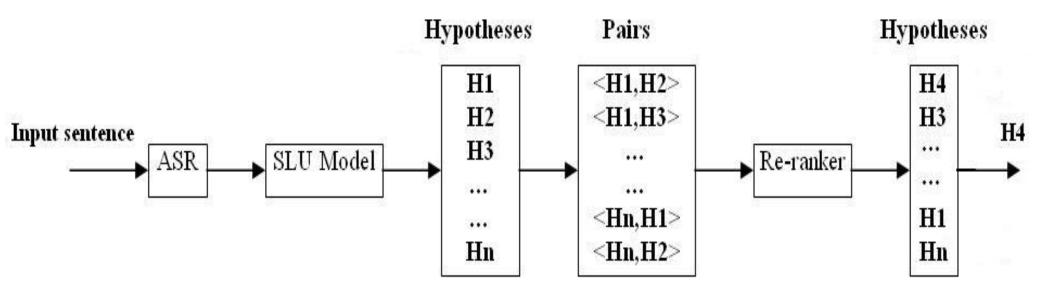


# **Re-ranking Model**

- The FST generates the most likely concept annotations.
- These are used to build annotation pairs,  $\langle s^i, s^j \rangle$ .
  - positive instances if s<sup>i</sup> more correct than s<sup>i</sup>,
- The trained binary classifier decides if s<sup>i</sup> is more accurate than s<sup>i</sup>.
- Each candidate annotation s<sup>i</sup> is described by a word sequence where each word is followed by its concept annotation.



## **Re-ranking framework**





### Example

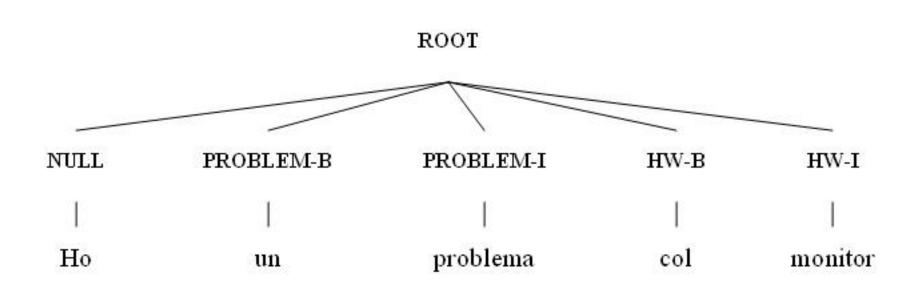
### I have a problem with the network card now

# s<sup>i</sup>: I NULL have NULL a NULL problem PROBLEM-B with NULL my NULL monitor HW-B

**s**: I **NULL** have **NULL** a **NULL** problem **HW-B** with **NULL** my **NULL** monitor

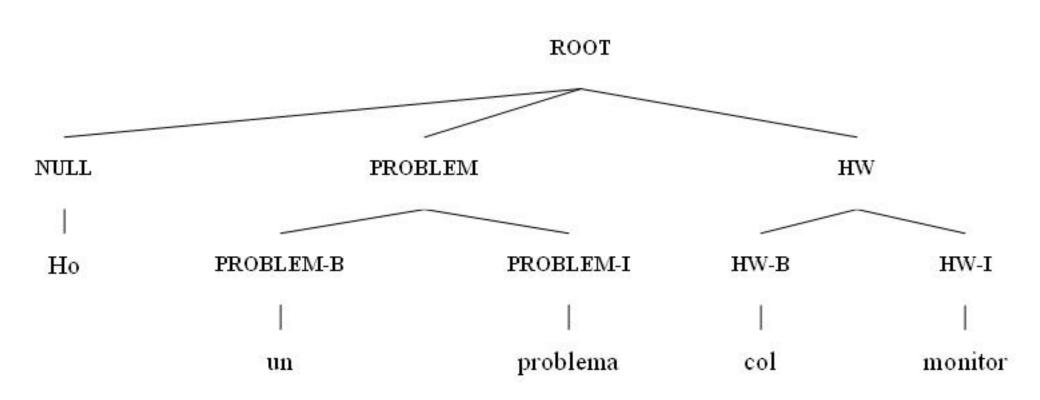


### Flat tree representation



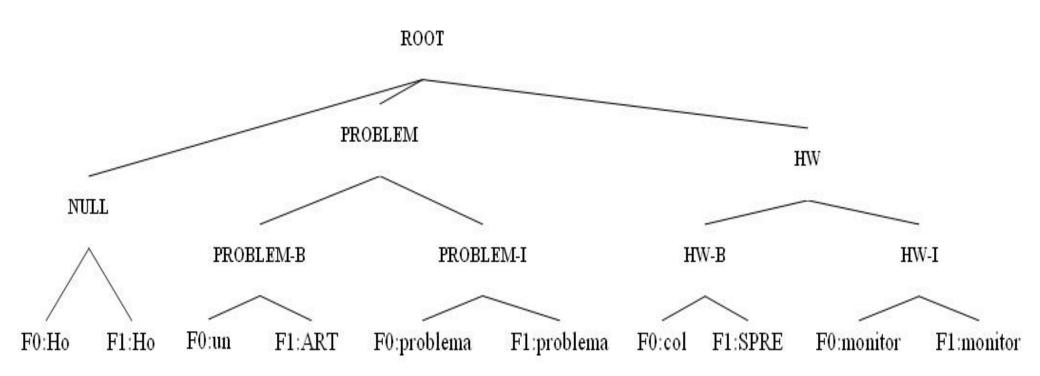


### **Multilevel Tree**





### **Enriched Multilevel Tree**





### Results

Model	Concept Error Rate				
≈ 30% of error reduction of					
FSA the best model 23.2					
FSA+Re-Ranking	16.01				



### **Structured Perceptron**

Training set  $(x_i, y_i)$  for  $i = 1 \dots n$ **Inputs:**  $\mathbf{W} = 0$ **Initialization:**  $F(x) = \operatorname{argmax}_{y \in \mathbf{GEN}(x)} \mathbf{\Phi}(x, y) \cdot \mathbf{W}$ **Define:** For t = 1 ... T, i = 1 ... n**Algorithm:**  $z_i = F(x_i)$ If  $(z_i \neq y_i)$   $\mathbf{W} = \mathbf{W} + \mathbf{\Phi}(x_i, y_i) - \mathbf{\Phi}(x_i, z_i)$ Parameters W **Output:** 

### Structured Output Prediction with Structural Support Vector Machines

**Thorsten Joachims** 

Cornell University Department of Computer Science

Joint work with

T. Hofmann, I. Tsochantaridis, Y. Altun (Brown/Google/TTI)T. Finley, R. Elber, Chun-Nam Yu, Yisong Yue, F. RadlinskiP. Zigoris, D. Fleisher (Cornell)

### Supervised Learning

• Assume: Data is i.i.d. from

P(X,Y)

• Given: Training sample

$$S = ((x_1, y_1), ..., (x_n, y_n))$$

• **Goal:** Find function from input space *X* to output space *Y* 

$$h: X \longrightarrow Y$$

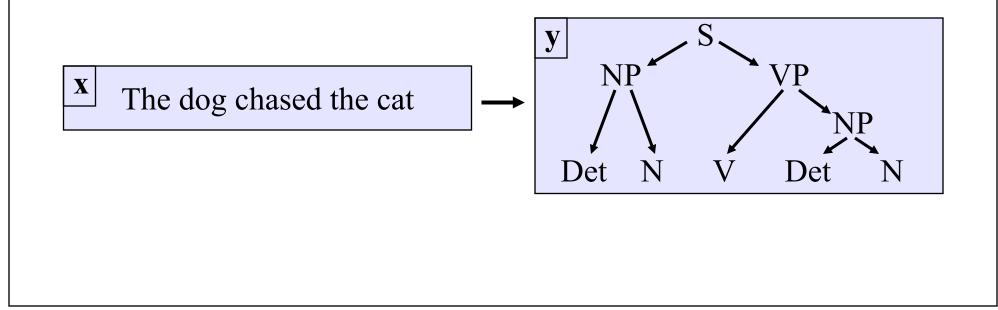
Complex objects

with low risk / prediction error

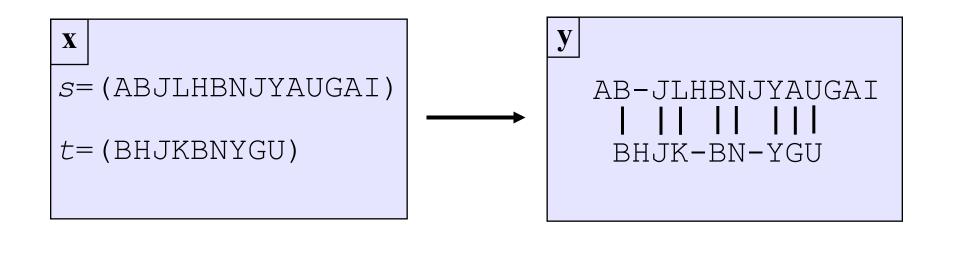
$$R(h) = \int \Delta(h(x), y) dP(X, Y)$$

• Methods: Kernel Methods, SVM, Boosting, etc.

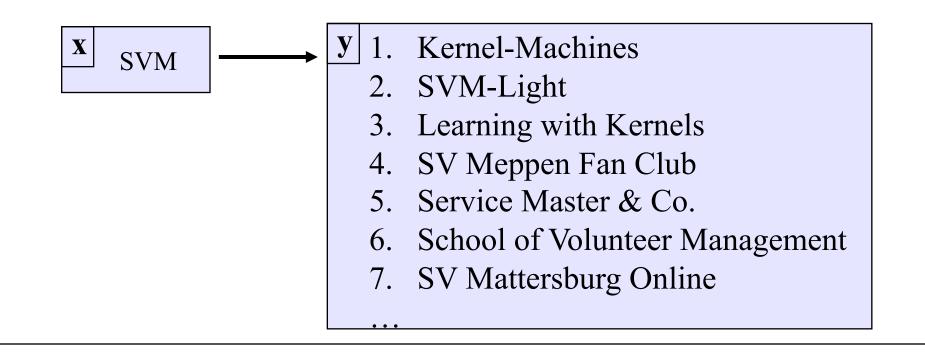
- Natural Language Parsing
  - Given a sequence of words *x*, predict the parse tree *y*.
  - Dependencies from structural constraints, since y has to be a tree.



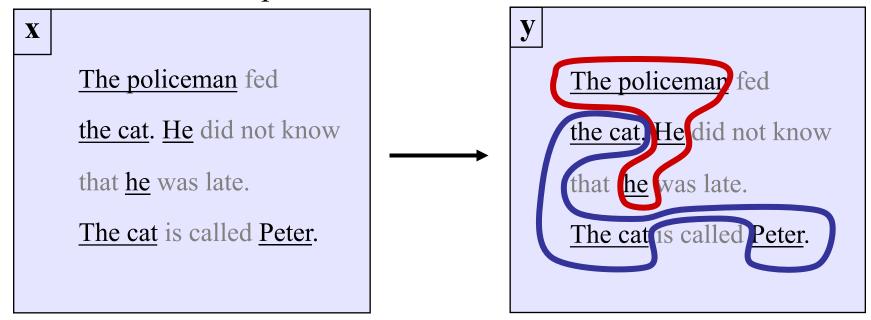
- Protein Sequence Alignment
  - Given two sequences x=(s,t), predict an alignment y.
  - Structural dependencies, since prediction has to be a valid global/local alignment.



- Information Retrieval
  - Given a query x, predict a ranking y.
  - Dependencies between results (e.g. avoid redundant hits)
  - Loss function over rankings (e.g. AvgPrec)



- Noun-Phrase Co-reference
  - Given a set of noun phrases *x*, predict a clustering *y*.
  - Structural dependencies, since prediction has to be an equivalence relation.
  - Correlation dependencies from interactions.



- and many many more:
  - Sequence labeling (e.g. part-of-speech tagging, named-entity recognition) [Lafferty et al. 01, Altun et al. 03]
  - Collective classification (e.g. hyperlinked documents) [Taskar et al. 03]
  - Multi-label classification (e.g. text classification) [Finley & Joachims 08]
  - Binary classification with non-linear performance measures (e.g. optimizing F1-score, avg. precision) [Joachims 05]
  - Inverse reinforcement learning / planning (i.e. learn reward function to predict action sequences) [Abbeel & Ng 04]

### Overview

• Task: Discriminative learning with complex outputs

### Related Work

- SVM algorithm for complex outputs
  - Predict trees, sequences, equivalence relations, alignments
  - General non-linear loss functions
  - Generic formulation as convex quadratic program
- Training algorithms
  - n-slack vs. 1-slack formulation
  - Correctness and sparsity bound
- Applications
- Sequence alignment for protein structure prediction [w/ Chun-Nam Yu]
- Diversification of retrieval results in search engines [w/ Yisong Yue]
- Supervised clustering [w/ Thomas Finley]
- Conclusions

### Why Discriminative Learning for Structured Outputs?

•	Imj	Precision/Recall Break-Even Point	Naïve Bayes	Linear SVM	it! er 06]
		Reuters	72.1	87.5	
•	Dir	WebKB	82.0	90.3	
	_	Ohsumed	62.4	71.6	ification

- Improve upon prediction accuracy of existing generative methods!
  - Natural language parsing: generative models like probabilistic contextfree grammars
  - SVM outperforms naïve Bayes for text classification [Joachims, 1998]
     [Dumais et al., 1998]
- More flexible models!
  - Avoid generative (independence) assumptions
  - Kernels for structured input spaces and non-linear functions

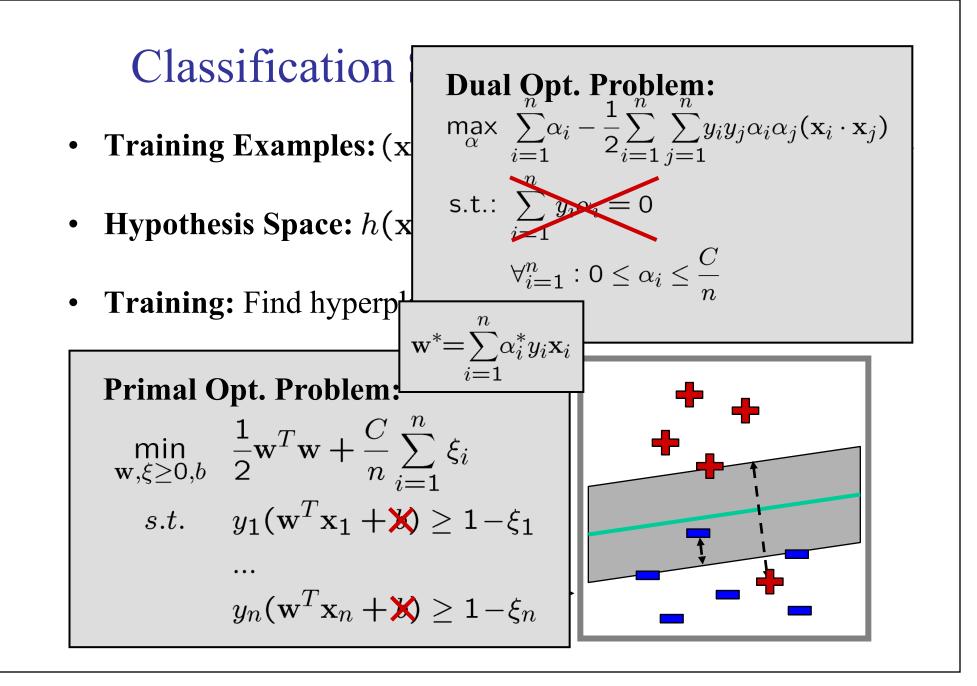
### Related Work

#### • Generative training (i.e. model P(Y,X))

- Hidden-Markov models
- Probabilistic context-free grammars
- Markov random fields
- etc.
- Discriminative training (i.e. model P(Y|X) or minimize risk)
  - Multivariate output regression [Izeman, 1975] [Breiman & Friedman, 1997]
  - Kernel Dependency Estimation [Weston et al. 2003]
  - Transformer networks [LeCun et al, 1998]
  - Conditional HMM [Krogh, 1994]
  - Conditional random fields [Lafferty et al., 2001]
  - Perceptron training of HMM [Collins, 2002]
  - Maximum-margin Markov networks [Taskar et al., 2003]
  - Structural SVMs [Altun et al. 03] [Joachims 03] [TsoHoJoAl04]

### Overview

- Task: Discriminative learning with complex outputs
- Related Work
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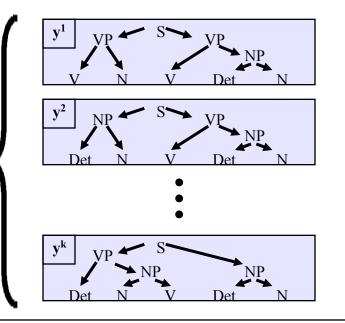
### Challenges in Discriminative Learning with Complex Outputs

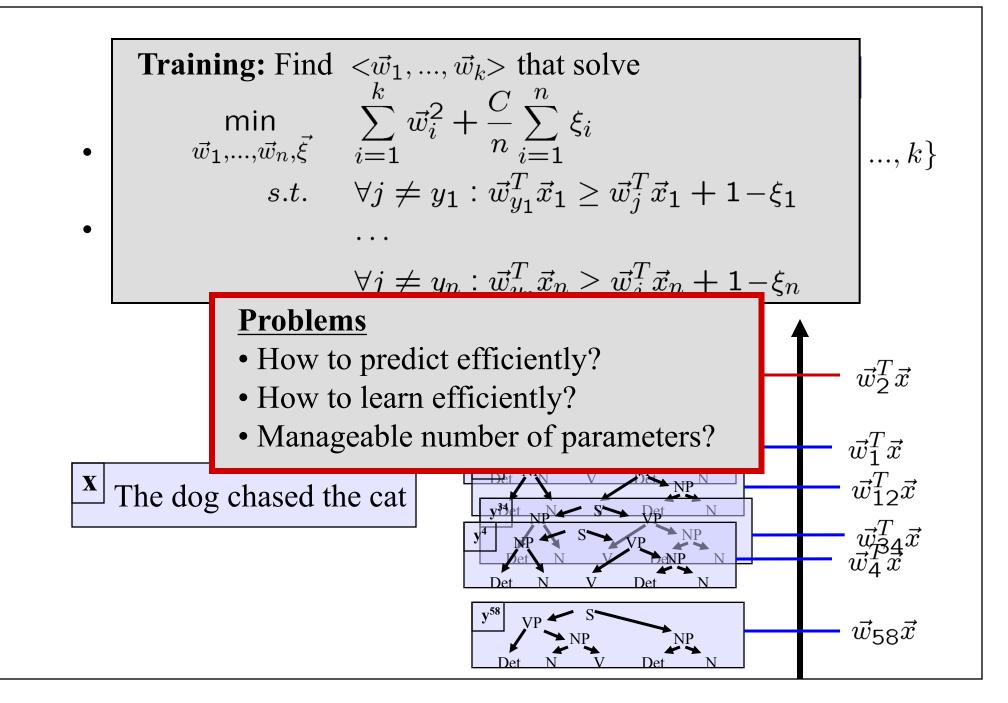
- Approach: view as multi-class classification task
  - Every complex output  $y^i \in Y$  is one class
- Problems:

X

- Exponentially many classes!
  - How to predict efficiently?
  - How to learn efficiently?
- Potentially huge model!
  - Manageable number of features?

The dog chased the cat





#### Joint Feature Map

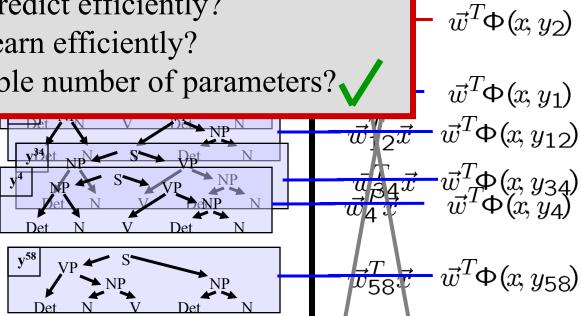
- Feature vector  $\Phi(x, y)$  that describes match between x and y
- Learn single weight vector and rank by  $\vec{w}^T \Phi(x, y)$

$$h(\vec{x}) = argmax_{y \in Y} \left[ \vec{w}^T \Phi(x, y) \right]$$

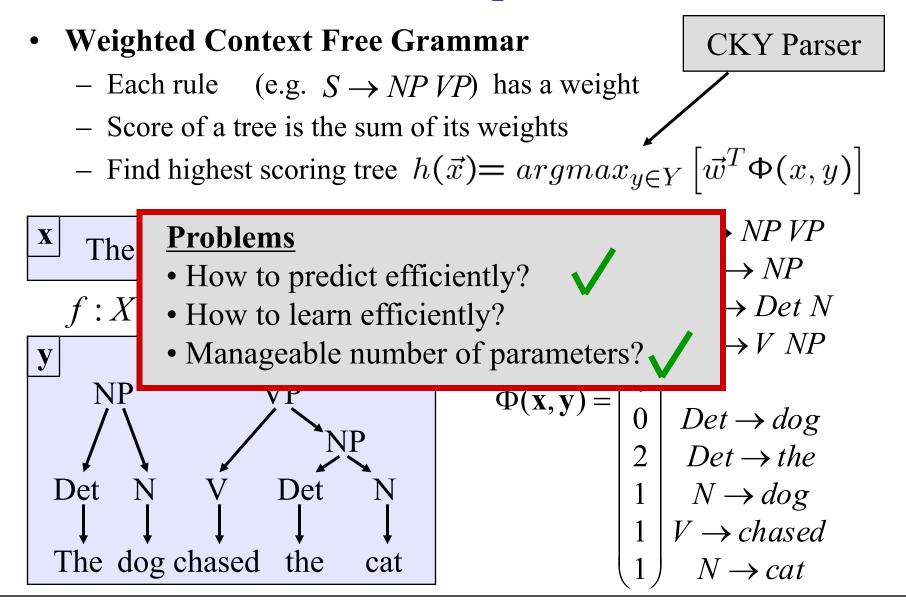
#### **Problems**

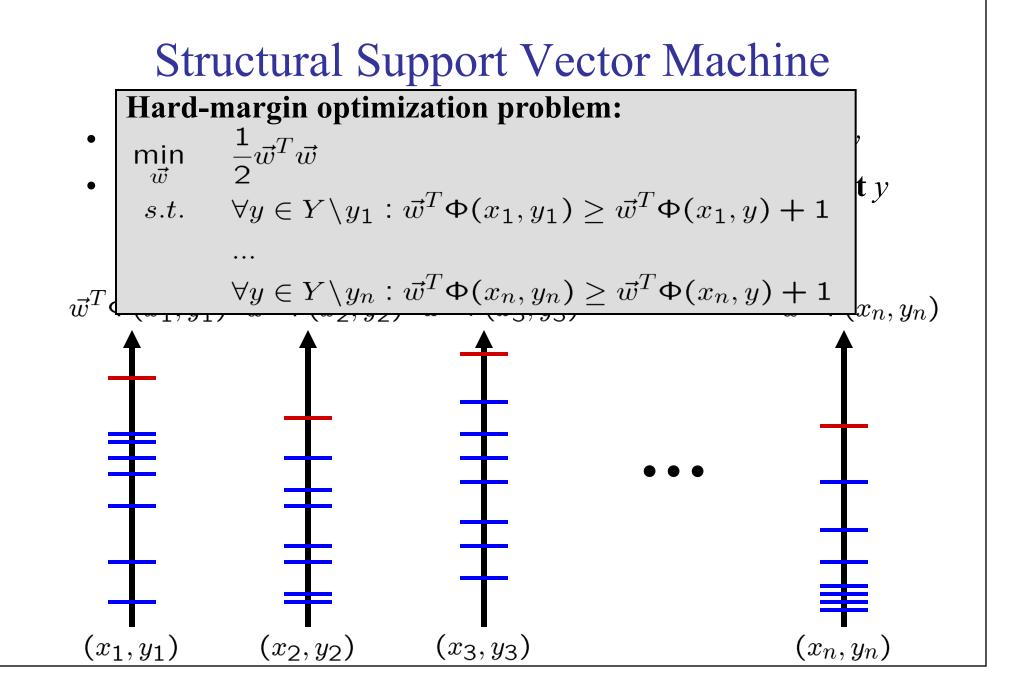
- How to predict efficiently?
- How to learn efficiently?
- Manageable number of parameters?

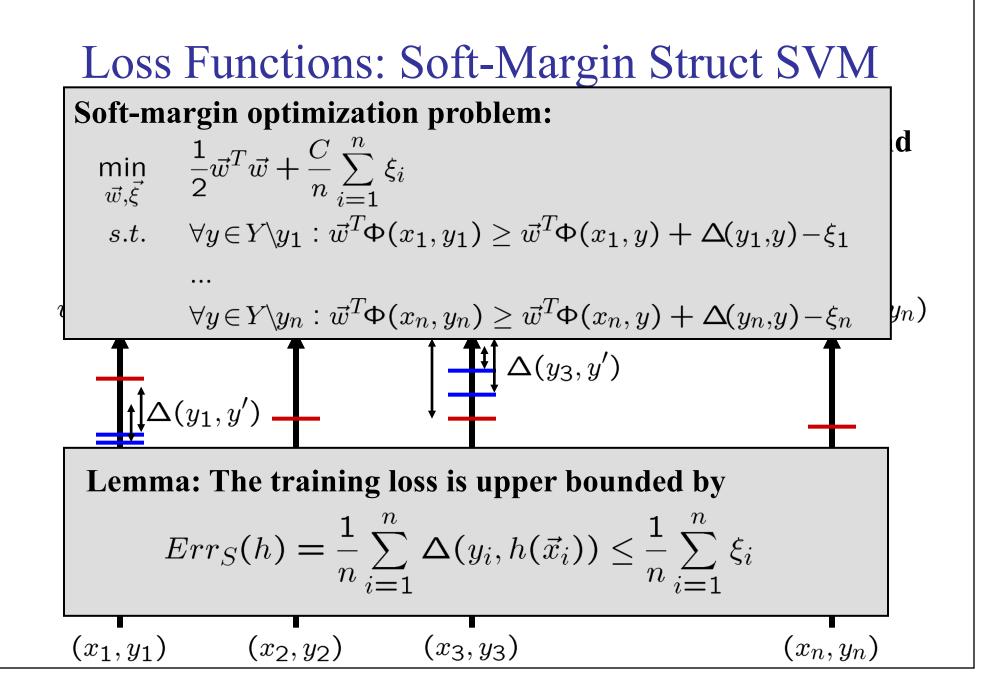
X The dog chased the cat



#### Joint Feature Map for Trees







### Experiment: Natural Language Parsing

#### • Implemention

- Incorporated modified version of Mark Johnson's CKY parser
- Learned weighted CFG with  $\epsilon = 0.01, C = 1$
- Data
  - Penn Treebank sentences of length at most 10 (start with POS)
  - Train on Sections 2-22: 4098 sentences
  - Test on Section 23: 163 sentences

	Test Accuracy		
Method	Acc	$F_1$	
PCFG with MLE	55.2	86.0	
SVM with $(1-F_1)$ -Loss	58.9	88.5	Ľ

[TsoJoHoAl04]

- more complex features [TaKlCoKoMa04]

### Generic Structural SVM

- Application Specific Design of Model
  - Loss function  $\Delta(y_i, y)$
  - Representation  $\Phi(x, y)$

→ Markov Random Fields [Lafferty et al. 01, Taskar et al. 04]

• Prediction:

$$\hat{y} = argmax_{y \in Y} \{ \vec{w}^T \Phi(x, y) \}$$

• Training:

$$\min_{\vec{w},\vec{\xi}\geq 0} \quad \frac{1}{2}\vec{w}^T\vec{w} + \frac{C}{n}\sum_{i=1}^n \xi_i \\ s.t. \quad \forall y \in Y \setminus y_1 : \vec{w}^T \Phi(x_1, y_1) \geq \vec{w}^T \Phi(x_1, y) + \Delta(y_1, y) - \xi_1 \\ \dots \\ \forall y \in Y \setminus y_n : \vec{w}^T \Phi(x_n, y_n) \geq \vec{w}^T \Phi(x_n, y) + \Delta(y_n, y) - \xi_n$$

• Applications: Parsing, Sequence Alignment, Clustering, etc.

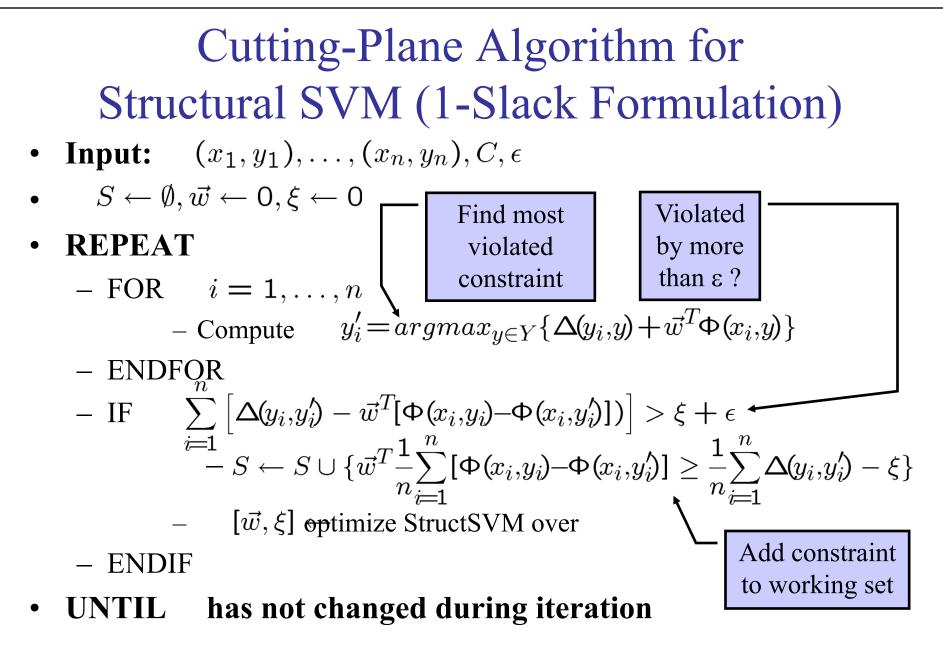
#### Reformulation of the Structural SVM QP

# [TsoJoHoAl04] **n-Slack Formulation:** $\min_{\vec{w},\vec{\xi}} \quad \frac{1}{2}\vec{w}^T\vec{w} + \frac{C}{n}\sum_{i=1}^n \xi_i$ s.t. $\forall y' \in Y : \vec{w}^T \Phi(x_1, y_1) - \vec{w}^T \Phi(x_1, y') \ge \Delta(y_1, y) - \xi_1$ $\forall y' \in Y : \vec{w}^T \Phi(x_n, y_n) - \vec{w}^T \Phi(x_n, y') \geq \Delta(y_n, y) - \xi_n$

#### Reformulation of the Structural SVM QP

#### **n-Slack Formulation:**

[TsoJoHoAl04]



[Jo06] [JoFinYu08]

### Polynomial Sparsity Bound

• **Theorem:** The cutting-plane algorithm finds a solution to the Structural SVM soft-margin optimization problem in the 1-slack formulation after adding at most

$$\left\lceil \log_2\left(\frac{\Delta}{4R^2C}\right) \right\rceil + \left\lceil \frac{16R^2C}{\varepsilon} \right\rceil$$

constraints to the working set S, so that the primal constraints are feasible up to a precision and the objective on S is optimal. The loss has to be bounded  $0 \le \Delta(y_i, y) \le \Delta$ , and  $2||\Phi(x,y)|| \le R$ .

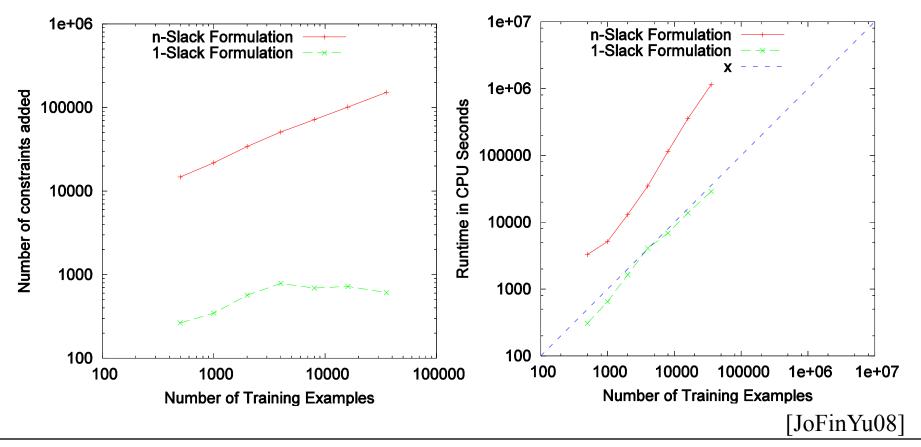
[Jo03] [Jo06] [TeoLeSmVi07] [JoFinYu08]

#### **Empirical Comparison: Different Formulations**

#### **Experiment Setup:**

- Part-of-speech tagging on Penn Treebank corpus

- ~36,000 examples, ~250,000 features in linear HMM model



### Applying StructSVM to New Problem

- General
  - SVM-struct algorithm and implementation

http://svmlight.joachims.org

- Theory (e.g. training-time linear in n)
- Application specific
  - Loss function  $\Delta(y_i, y)$
  - Representation  $\Phi(x, y)$
  - Algorithms to compute  $\hat{y} = argmax_{y \in Y} \{ \vec{w}^T \Phi(x_i, y) \}$   $\hat{y} = argmax_{y \in Y} \{ \Delta(y_i, y) + \vec{w}^T \Phi(x_i, y) \}$
- Properties
  - General framework for discriminative learning
  - Direct modeling, not reduction to classification/regression
  - "Plug-and-play"

### Overview

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  - Supervised clustering [w/ Thomas Finley]
- Conclusions

Comparative Modeling of Protein Structure

• Goal: Predict structure from sequence

h("APPGEAYLQV")  $\rightarrow$ 

Contraction of the second

- Hypothesis:
  - Amino Acid sequences for into structure with lowest energy
  - Problem: Huge search space (>  $2^{100}$  states)
- Approach: Comparative Modeling
  - − Similar protein sequences fold into similar shapes
     → use known shapes as templates
  - Task 1: Find a similar known protein for a new protein
     h("APPGEAYLQV", → yes/no
- → Task 2: Map new protein into known structure h("APPGEAYLQV",  $\checkmark$  ) → [A→3,P→4,P→7,...]
  - Task 3: Refine structure

[Jo03, JoElGa05, YuJoEl06]

#### Linear Score Sequence Alignment

#### Method: Find alignment y that maximizes linear score

$$y = argmax_{y \in Y} \{score(x=(s,t), y)\}$$

#### **Example:**

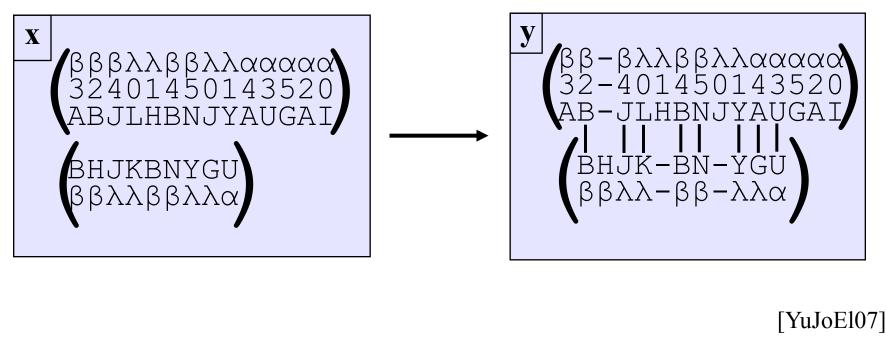
A

– Sequences:		A	В	С	D	-	
s = (A B C D)	A	10		-5	-10	-5	
t = (B A C C)	В	0		5	-10	-5	
	С		5		-10	-5	
- Alignment y <sub>1</sub> :	D		-10			-5	
A B C D	-	-5	-5	-5	-5	-5	
B A C C $\rightarrow score(x=(s,t),y_l) = 0 + 0 + 10 - 10 = 0$							
– Alignment y <sub>2</sub> :							
– A B C D							
BACC- $\rightarrow$ score	x = (s	$(,t),y_2)$	) = -5	+10-	+5+10	D-5 = 1	
lgorithm: Solve argmax via dynamic programming.							

### Predicting an Alignment

**Protein Sequence to Structure Alignment (Threading)** 

- Given a pair x=(s,t) of new sequence *s* and known structure *t*, predict the alignment *y*.
- Elements of *s* and *t* are described by features, not just character identity.



#### Scoring Function for Vector Sequences

**General form of linear scoring function:** 

score (x=(s,t),y) = 
$$\sum_{i} score(y_{i}^{s}, y_{i}^{t})$$
  
=  $\sum_{i} \mathbf{w}^{T} \phi(s, t, y_{i})$   
=  $\mathbf{w}^{T} \sum_{i} \phi(s, t, y_{i})$   
=  $\mathbf{w}^{T} \Phi(\mathbf{x}, \mathbf{y})$ 

- $\rightarrow$  match/gap score can be arbitrary linear function
- → argmax can still be computed efficiently via dynamic programming

#### **Estimation:**

- Generative estimation (e.g. log-odds, hidden Markov model)
- Discriminative estimation via structural SVM

### Loss Function and Separation Oracle

- Loss function:  $\Delta(y_i, y)$ 
  - Q loss: fraction of incorrect alignments

• Correct alignment 
$$\mathbf{y} = \begin{bmatrix} - & A & B & C & D \\ B & A & C & C & - \end{bmatrix}$$
  
• Alternate alignment  $\mathbf{y}' = \begin{bmatrix} A & - & B & C & D \\ B & A & C & C & - \end{bmatrix}$   
• Alternate alignment  $\mathbf{y}' = \begin{bmatrix} A & - & B & C & D \\ B & A & C & C & - \end{bmatrix}$ 

- Q4 loss: fraction of incorrect alignments outside window
  - Correct alignment  $\mathbf{y} = \begin{bmatrix} & A & B & C & D \\ B & A & C & C & \end{bmatrix}$ • Alternate alignment  $\mathbf{y}' = \begin{bmatrix} A & - & B & C & D \\ B & A & C & C & - \end{bmatrix}$ • Alternate alignment  $\mathbf{y}' = \begin{bmatrix} A & - & B & C & D \\ B & A & C & C & - \end{bmatrix}$

• Separation oracle:  $\hat{y} = argmax_{y \in Y} \{ \Delta(y_i, y) + \vec{w}^T \Phi(x_i, y) \}$ 

- Same dynamic programming algorithms as alignment

### Experiment

- Train set [Qiu & Elber]:
  - 5119 structural alignments for training, 5169 structural alignments for validation of regularization parameter C
- Test set:
  - 29764 structural alignments from new deposits to PDB from June 2005 to June 2006.
  - All structural alignments produced by the program CE by superimposing the 3D coordinates of the proteins structures. All alignments have CE Z-score greater than 4.5.
- Features (known for structure, SABLE predictions for sequence):
  - Amino acid identity (A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y)
  - Secondary structure  $(\alpha,\beta,\lambda)$
  - Exposed surface area (0,1,2,3,4,5)

#### **Experiment Results**

#### Models:

- Simple:  $\Phi(s,t,y_i) \Leftrightarrow (A|A; A|C; ...;-|Y; \alpha|\alpha; \alpha|\beta...; 0|0; 0|1;...)$
- Anova2:  $\Phi(s,t,y_i) \Leftrightarrow (A\alpha | A\alpha ...; \alpha 0 | \alpha 0 ...; A0 | A0;...)$
- **Tensor:**  $\Phi(s,t,y_i) \Leftrightarrow (A\alpha 0 | A\alpha 0; A\alpha 0 | A\alpha 1; ...)$

#### Ability to train complex models?

Q-Score	# Features	Test		
Simple	1020	39.89		
Anova2	49634	44.98		
Tensor	203280	42.81		
Window	447016	46.30		
Q-score when optimizing to Q-loss				

Q4-score	Test	
BLAST	28.44	
SVM (Window)	70.71	
SSALN [QiuElber]	67.30	
TM-align [ZhaSko]	(85.32)	
O4-score when optimizing to $O4$ -loss		

**Comparison against other methods?** 

Q4-score when optimizing to Q4-loss

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### **Diversified Retrieval**

#### • Ambiguous queries:

- Example query: "SVM"
  - ML method
  - Service Master Company
  - Magazine
  - School of veterinary medicine
  - Sport Verein Meppen e.V.
  - SVM software
  - SVM books
- "submodular" performance measure
  - → make sure each user gets at least one relevant result
- Learning Queries:
  - Find all information about a topic
  - Eliminate redundant information

Query: SVM

- 1. Kernel Machines
- 2. SVM book
- 3. SVM-liaht

5.

6.

7.

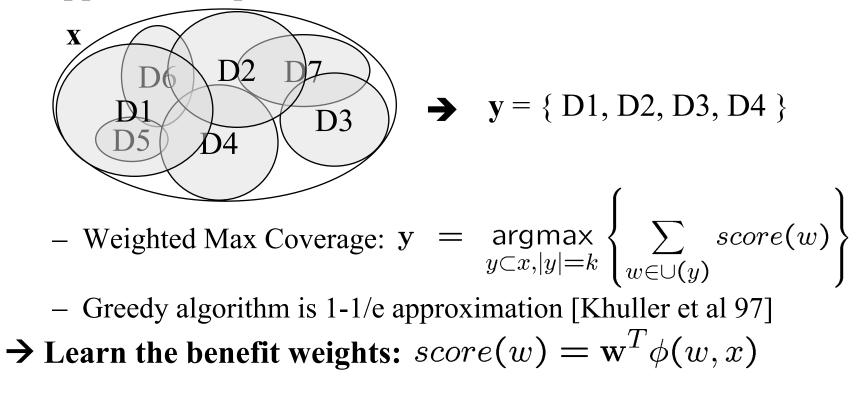
- 4. Query: SVM
  - 1. Kernel Machines
  - 2. Service Master Co
  - 3. SV Meppen
  - 4. UArizona Vet. Med.
  - 5. SVM-light
  - 6. Intro to SVM

7. .

[YueJo08]

## Approach

- Prediction Problem:
  - Given set  $\mathbf{x}$ , predict size k subset  $\mathbf{y}$  that satisfies most users.
- Approach: Topic Red. 1/4 Word Red. [SwMaKi08]



[YueJo08]

### Features Describing Word Importance

#### • How important is it to cover word w

- w occurs in at least X% of the documents in x
- w occurs in at least X% of the titles of the documents in x
- w is among the top 3 TFIDF words of X% of the documents in  $\boldsymbol{x}$
- w is a verb
- → Each defines a feature in  $\phi(w, x)$
- How well a document d covers word w
  - w occurs in d
  - w occurs at least k times in d
  - w occurs in the title of d
  - w is among the top k TFIDF words in d
  - $\rightarrow$  Each defines a separate vocabulary and scoring function

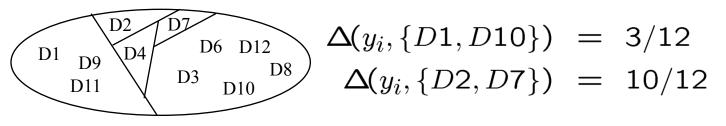


#### Loss Function and Separation Oracle

- Loss function:  $\Delta(y_i, y)$ 
  - Popularity-weighted percentage of subtopics not covered in y

 $\rightarrow$  More costly to miss popular topics

– Example:



- Separation oracle:  $\hat{y} = argmax_{y \in Y} \{ \Delta(y_i, y) + \vec{w}^T \Phi(x_i, y) \}$ 
  - Again a weighted max coverage problem

 $\rightarrow$  add artificial word for each subtopic with percentage weight

- Greedy algorithm is 1-1/e approximation [Khuller et al 97]

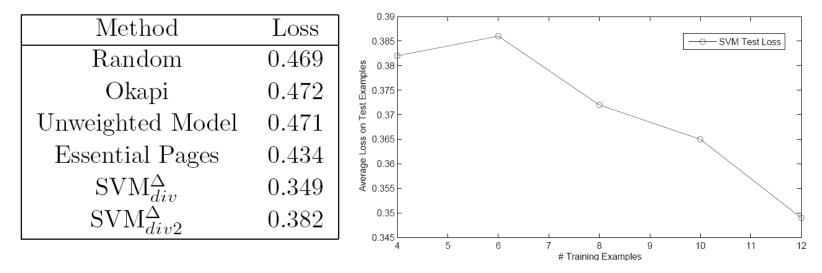
[YueJo08]

### Experiments

#### • Data:

- TREC 6-8 Interactive Track
- Relevant documents manually labeled by subtopic
- 17 queries (~700 documents), 12/4/1 training/validation/test
- Subset size k=5, two feature sets (div, div2)

#### • Results:

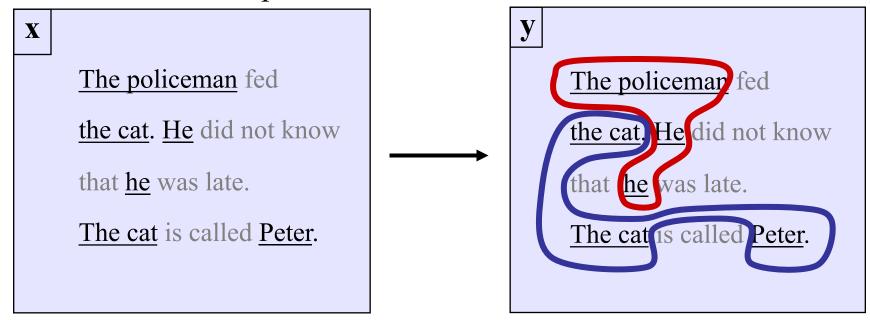


### Overview

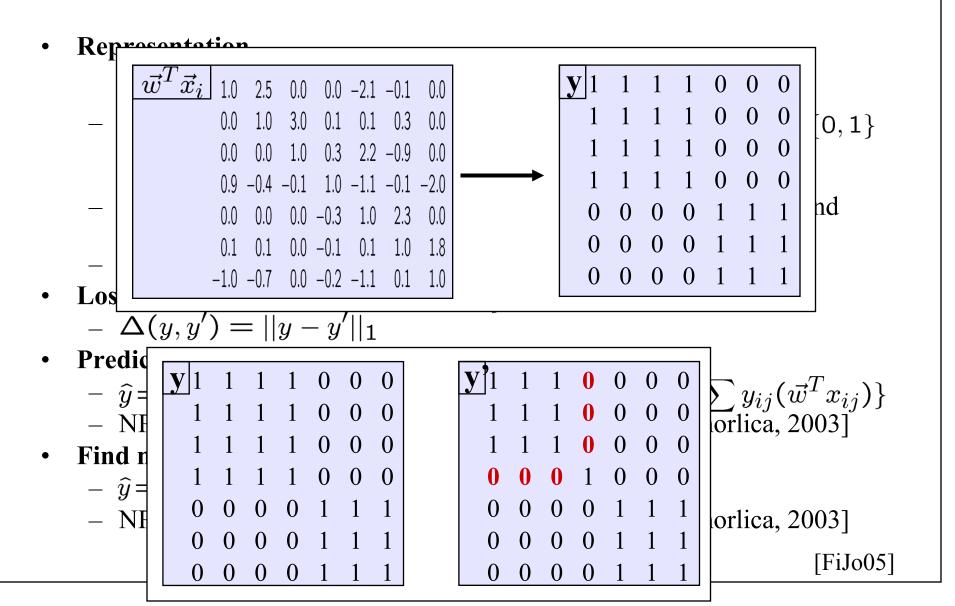
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### Learning to Cluster

- Noun-Phrase Co-reference
  - Given a set of noun phrases *x*, predict a clustering *y*.
  - Structural dependencies, since prediction has to be an equivalence relation.
  - Correlation dependencies from interactions.



#### Struct SVM for Supervised Clustering



### Summary and Conclusions

- Learning to predict complex output
  - Directly model machine learning application end-to-end
- An SVM method for learning with complex outputs
  - General method, algorithm, and theory
  - Plug in representation, loss function, and separation oracle
  - More details and further work:
    - Diversified retrieval [Yisong Yue, ICML08]
    - Sequence alignment [Chun-Nam Yu, RECOMB07, JCB08]
    - Supervised k-means clustering [Thomas Finley, forthcoming]
    - Approximate inference and separation oracle [Thomas Finley, ICML08]
    - Efficient kernelized structural SVMs [Chun-Nam Yu, KDD08]

#### • Software: SVM<sup>struct</sup>

- General API
- Instances for sequence labeling, binary classification with non-linear loss, context-free grammars, diversified retrieval, sequence alignment, ranking
- http://svmlight.joachims.org/

# PART II: Basics of Natural Language Processing



# Part-of-Speech tagging

Given a sentence W<sub>1</sub>...W<sub>n</sub> and a tagset of lexical categories, find the most likely tag T<sub>1</sub>...T<sub>n</sub> for each word in the sentence

#### Example

Secretariat/NNP is/VBZ expected/VBN to/TO race/VB tomorrow/NN People/NNS continue/VBP to/TO inquire/VB the/DT reason/NN for/IN the/DT race/NN for/IN outer/JJ space/NN

Note that many of the words may have unambiguous tags

But enough words are either ambiguous or unknown that it's a nontrivial task



# Part Of Speech (POS) Tagging

- Annotate each word in a sentence with a part-ofspeech.
  - I ate the spaghetti with meatballs.
  - Pro V Det N Prep N
  - John saw the saw and decided to take itto the table.PNVDetNConVPart VProProp DetN
- Useful for subsequent syntactic parsing and word sense disambiguation.



# PTB Tagset (36 main tags + punctuation

### tags)

СС Coordinating conjunction CD Cardinal number DТ Determiner ΕХ Existential there FΨ Foreign word Preposition or subordinating conjunction IN JJ Adjective Adjective, comparative JJR. JJS Adjective, superlative LS List item marker MD. Modal NN Noun, singular or mass NNS. Noun, plural NP. Proper noun, singular Proper noun, plural NPS PDT Predeterminer POS Possessive ending PP Personal pronoun PP\$ Possessive pronoun RB Adverb RBR Adverb, comparative Adverb, superlative RBS RP Particle SYM Symbol TO toUH Interjection VB. Verb, base form VBD Verb, past tense VBG Verb, gerund or present participle VBN. Verb, past participle VBP Verb, non-3rd person singular present VBZ. Verb, 3rd person singular present Wh-determiner WDT WP Wh-pronoun Possessive wh-pronoun WP\$

WRB Wh-adverb

# Solution

- Text Classifier:
  - Tags categories
  - Features windows of words around the target word
  - N-grams



# **Named Entity Recognition**

- NE involves identification of proper names in texts, and classification into a set of predefined categories of interest.
- Three universally accepted categories: person, location and organisation
- Other common tasks: recognition of date/time expressions, measures (percent, money, weight etc), email addresses etc.
- Other domain-specific entities: names of drugs, medical conditions, names of ships, bibliographic references etc.

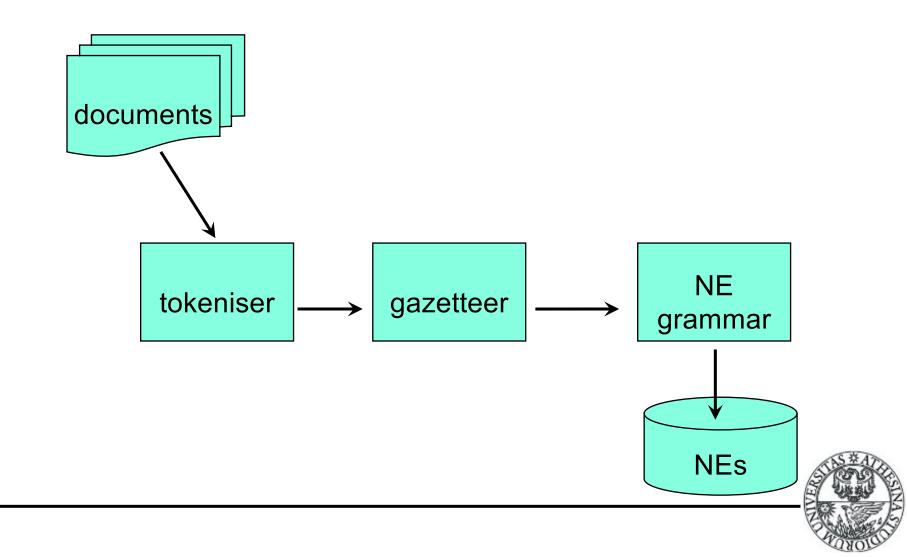


#### **Problems in NE Task Definition**

- Category definitions are intuitively quite clear, but there are many grey areas.
- Many of these grey area are caused by metonymy.
  - Organisation vs. Location : "England won the World Cup" vs. "The World Cup took place in England".
  - Company vs. Artefact: "shares in MTV" vs. "watching MTV"
  - Location vs. Organisation: "she met him at Heathrow" vs. "the Heathrow authorities"



### **NE System Architecture**



#### Approach con't

- Again Text Categorization
- N-grams in a window centered on the NER
- Additional Features
  - Gazetteer
  - Word Capitalize
  - Beginning of the sentence
  - Is it all capitalized



#### Approach con't

- NE task in two parts:
  - Recognising the entity boundaries
  - Classifying the entities in the NE categories
- Some work is only on one task or the other
- Tokens in text are often coded with the IOB scheme
  - O outside, B-XXX first word in NE, I-XXX all other words in NE
  - Easy to convert to/from inline MUC-style markup

Argentina	<b>B-LOC</b>
played	0
with	0
Del	<b>B-PER</b>
Bosque	I-PER

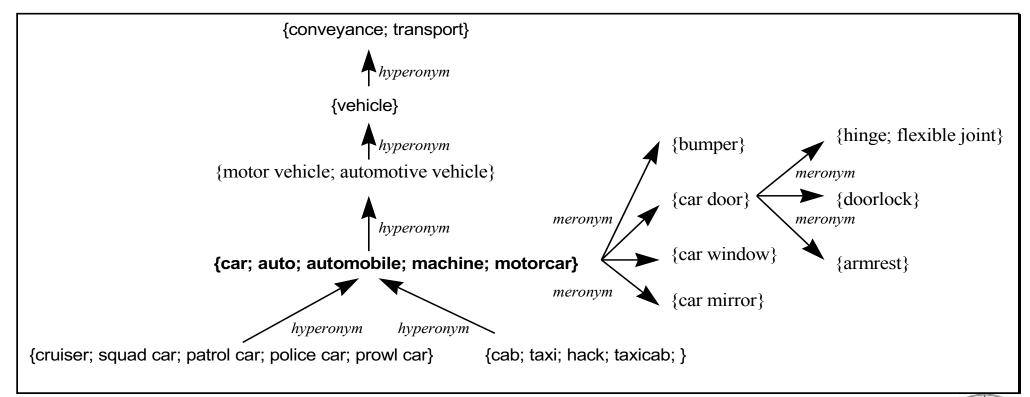


#### WordNet

- Developed at Princeton by George Miller and his team as a model of the mental lexicon.
- Semantic network in which concepts are defined in terms of relations to other concepts.
- Structure:
  - organized around the notion of synsets (sets of synonymous words)
  - basic semantic relations between these synsets
  - Initially no glosses
  - Main revision after tagging the Brown corpus with word meanings: SemCor.
  - http://www.cogsci.princeton.edu/~wn/w3wn.html



#### Structure





#### **Syntactic Parsing**

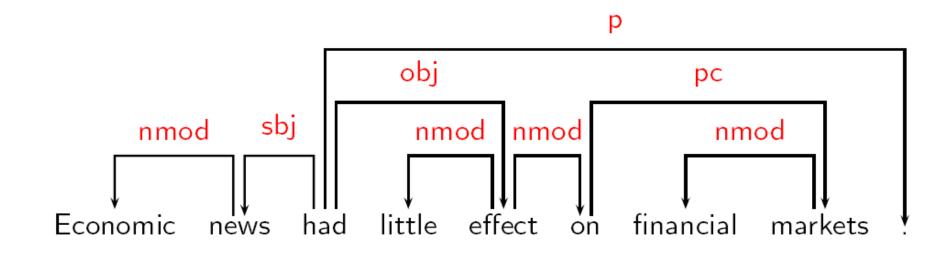


#### **Dependency Syntax**

- ► The basic idea:
  - Syntactic structure consists of lexical items, linked by binary asymmetric relations called dependencies.



#### **Dependency Structure**





#### Terminology

÷

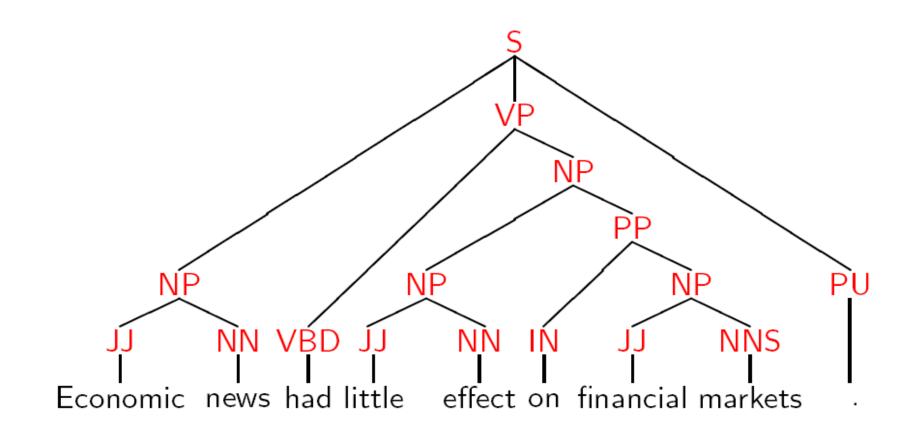
Superior	Inferior
Head	Dependent
Governor	Modifier
Regent	Subordinate

÷



#### **Phrase Structure**

#### (or Constituent Structure)





#### Comparison

Dependency structures explicitly represent

- head-dependent relations (directed arcs),
- functional categories (arc labels),
- possibly some structural categories (parts-of-speech).
- Phrase structures explicitly represent
  - phrases (nonterminal nodes),
  - structural categories (nonterminal labels),
  - possibly some functional categories (grammatical functions).
- Hybrid representations may combine all elements.



#### **Predicate Argument Structures**



# Shallow semantics from predicate argument structures

#### In an event:

- target words describe relation among different entities
- the participants are often seen as predicate's arguments.
- Example:

a phosphor gives off electromagnetic energy in this form



# Shallow semantics from predicate argument structures

#### In an event:

- target words describe relation among different entities
- the participants are often seen as predicate's arguments.
- Example:

[ <sub>Arg0</sub> a phosphor] [ <sub>predicate</sub> gives off] [ <sub>Arg1</sub> electromagnetic energy] [ <sub>ArgM</sub> in this form]



# Shallow semantics from predicate argument structures

#### In an event:

- target words describe relation among different entities
- the participants are often seen as predicate's arguments.
- Example:

[ Arg0 a phosphor] [ predicate gives off] [ Arg1 electromagnetic energy] [ ArgM in this form] [ ARGM When] [ predicate hit] [ Arg0 by electrons] [ Arg1 a phosphor]



#### Example on Predicate Argument Classification

- In an event:
  - target words describe relation among different entities
  - the participants are often seen as predicate's arguments.
- Example:

Paul gives a talk in Rome



#### Example on Predicate Argument Classification

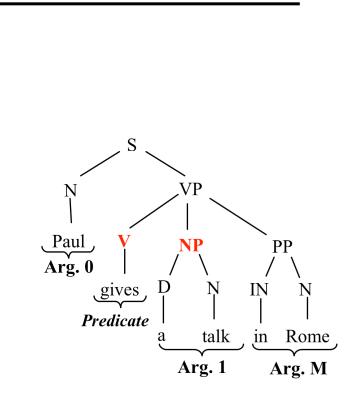
- In an event:
  - target words describe relation among different entities
  - the participants are often seen as predicate's arguments.
- Example:
  - [ Arg0 Paul] [ predicate gives ] [ Arg1 a talk] [ ArgM in Rome]



#### Predicate-Argument Feature Representation

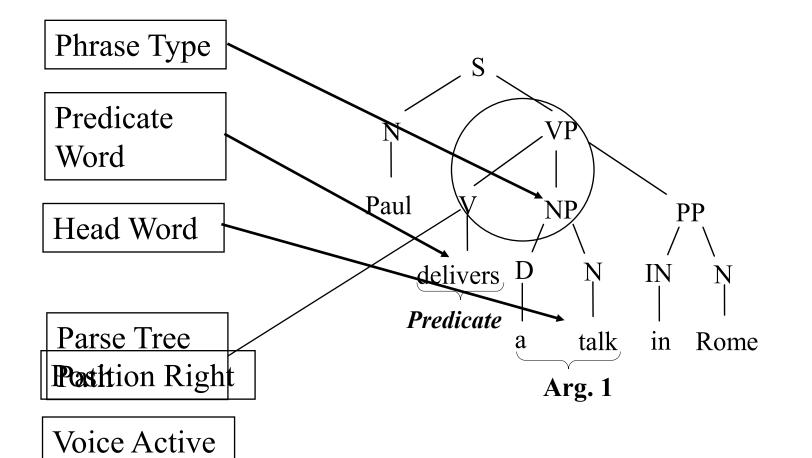
Given a sentence, a predicate *p*:

- 1. Derive the sentence parse tree
- 2. For each node pair  $\langle N_p, N_x \rangle$ 
  - a. Extract a feature representation set
  - b. If  $N_x$  exactly covers the Arg-*i*, *F* is one of its positive examples
  - c. F is a negative example otherwise





#### **Vector Representation for the linear kernel**

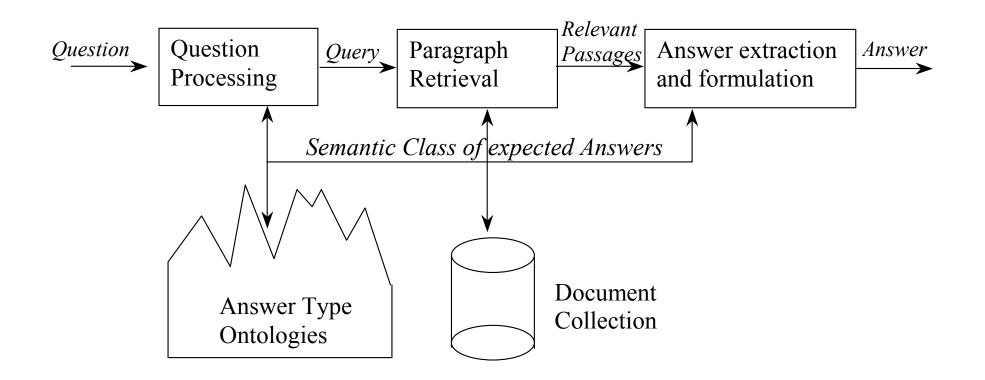




#### **Question Answering**



#### **Basic Pipeline**





#### **Question Classification**

- **Definition**: What does HTML stand for?
- Description: What's the final line in the Edgar Allan Poe poem "The Raven"?
- **Entity**: What foods can cause allergic reaction in people?
- **Human**: Who won the Nobel Peace Prize in 1992?
- **Location**: Where is the Statue of Liberty?
- Manner: How did Bob Marley die?
- **Numeric**: When was Martin Luther King Jr. born?
- Organization: What company makes Bentley cars?



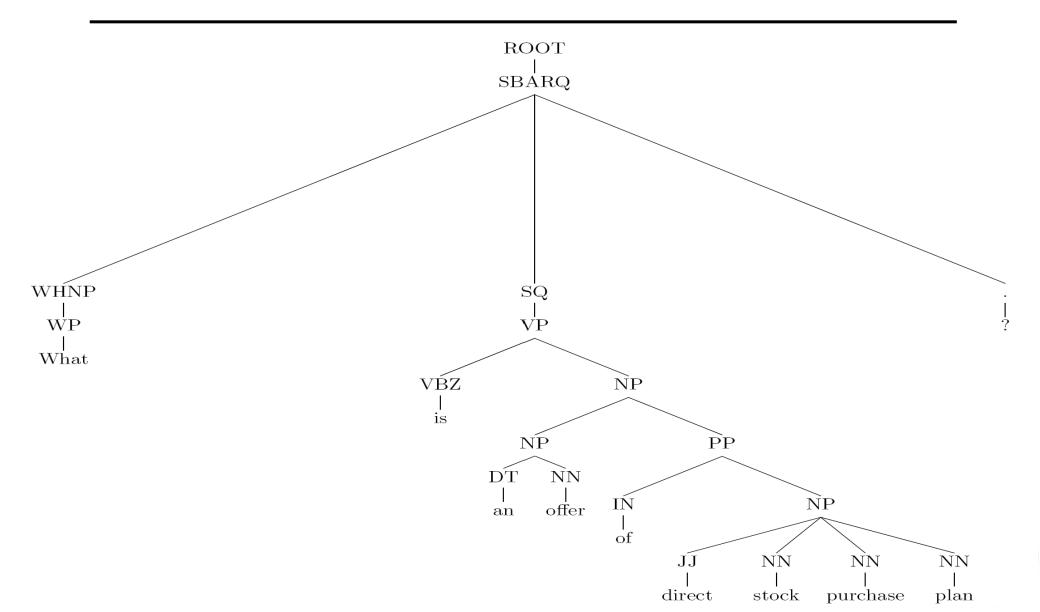
#### **Question Classifier based on Tree Kernels**

- Question dataset (http://l2r.cs.uiuc.edu/~cogcomp/Data/QA/QC/)
   [Lin and Roth, 2005])
  - Distributed on 6 categories: Abbreviations, Descriptions, Entity, Human, Location, and Numeric.
- Fixed split 5500 training and 500 test questions
- Using the whole question parse trees
  - Constituent parsing
  - Example

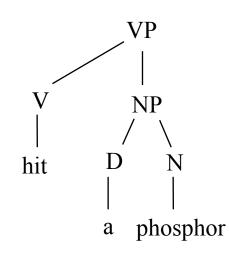
"What is an offer of direct stock purchase plan ?"



#### Syntactic Parse Trees (PT)

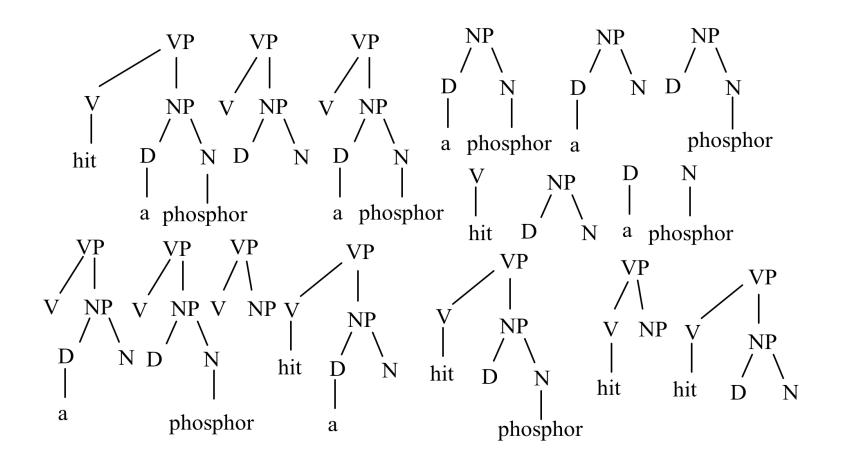


### Similarity based on the number of common substructures



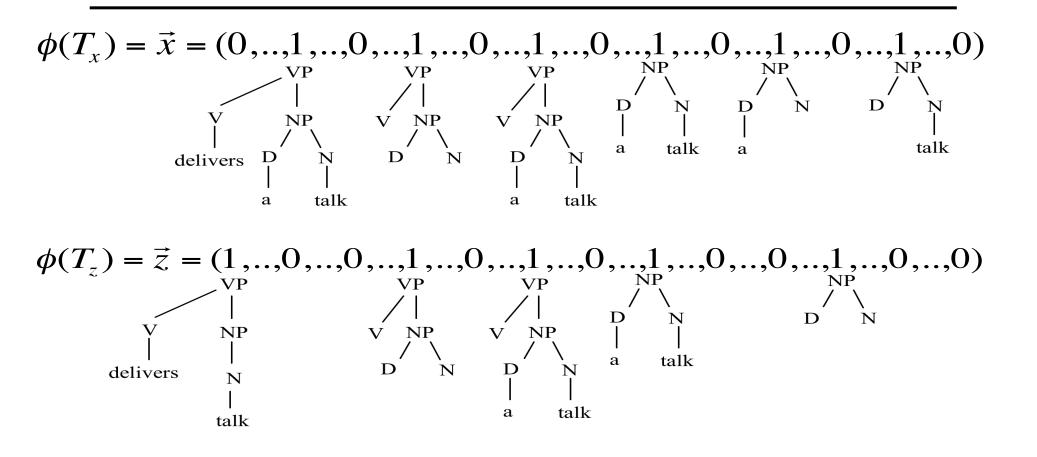


#### A portion of the substructure set





#### **Explicit tree fragment space**



•  $\vec{\chi} \cdot \vec{z}$  counts the number of common substructures



#### Similarity based on WordNet

Inverted Path Length:

$$sim_{IPL}(c_1, c_2) = \frac{1}{(1 + d(c_1, c_2))^{\alpha}}$$

Wu & Palmer:

$$sim_{WUP}(c_1, c_2) = \frac{2 dep(lso(c_1, c_2))}{d(c_1, lso(c_1, c_2)) + d(c_2, lso(c_1, c_2)) + 2 dep(lso(c_1, c_2))}$$

Resnik:

$$sim_{RES}(c_1, c_2) = -\log P(lso(c_1, c_2))$$

Lin:

$$sim_{LIN}(c_1, c_2) = \frac{2 \log P(lso(c_1, c_2))}{\log P(c_1) + \log P(c_2)}$$

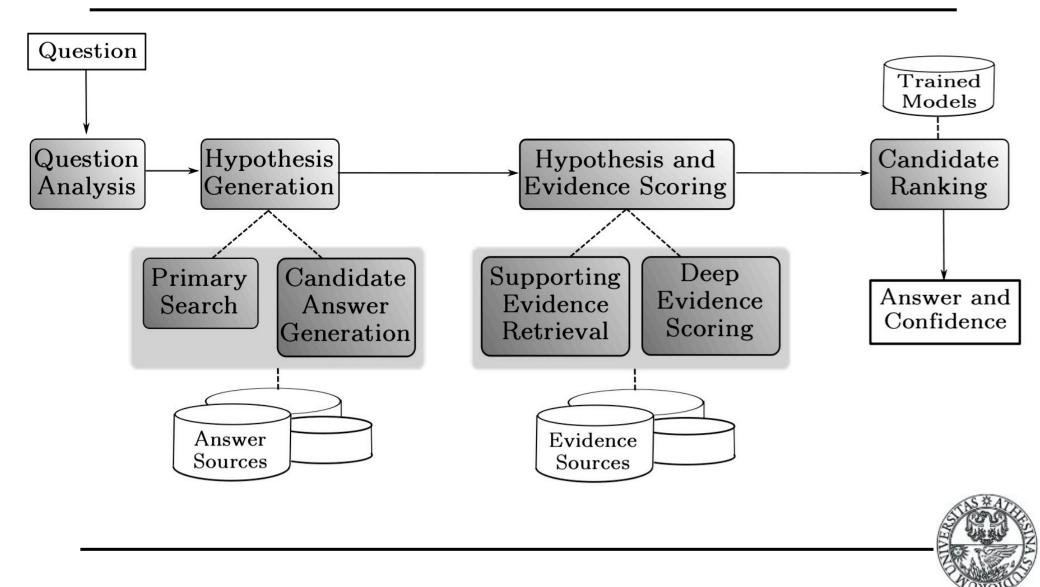


#### **Question Classification with SSTK**

	Accuracy					
$\lambda$ parameter	0.4	0.05	0.01	0.005	0.001	
linear (bow)	0.905					
string matching	0.890	0.910	0.914	0.914	0.912	
full	0.904	0.924	0.918	0.922	0.920	
full-ic	0.908	0.922	0.916	0.918	0.918	
path-1	0.906	0.918	0.912	0.918	0.916	
path-2	0.896	0.914	0.914	0.916	0.916	
lin	0.908	0.924	0.918	0.922	0.922	
wup	0.908	0.926	0.918	0.922	0.922	



#### A QA Pipeline: Watson Overview



### Thank you



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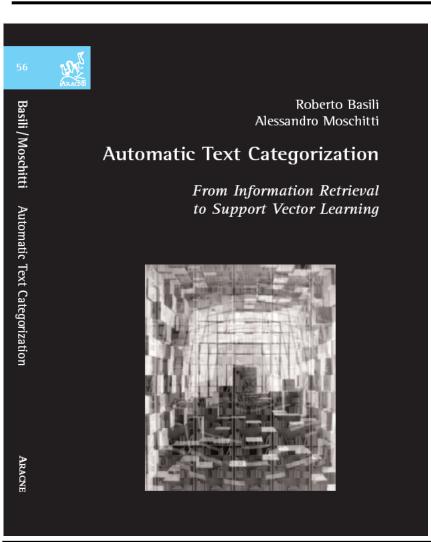
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