

# kLog

## A Language for Logical and Relational Learning with Kernels

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- Currently embedded in Prolog
- Four simple concepts:
  - Learning from interpretations
  - Entity/relationship data modeling
  - Deductive databases
  - Graph kernels

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- Make it possible to define in the same framework several kinds of **learning problems** ranging from plain classification and regression to entity classification to (hyper)link prediction and even unsupervised learning
- Modularity and **separation of concerns**:
  - Plug-in different graph kernels to create actual features
  - Plug-in different statistical, inference, optimization techniques
  - Simple semantics: the meaning of a kLog script only defines the learning problem and the associated features

# Supervised learning: A quite general formulation

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$$F(x, y) = w' \phi(x, y)$$

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- $F(x, y)$  measures the *compatibility* between  $x$  and  $y$
- Predictions can be obtained as

$$f(x) = \arg \max_y F(x, y)$$

This “inference” step is intractable in general (depending on the structure of the interdependencies between variables)

## **Propositional**

Naïve Bayes

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SVM-HMM

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# A classic trilogy

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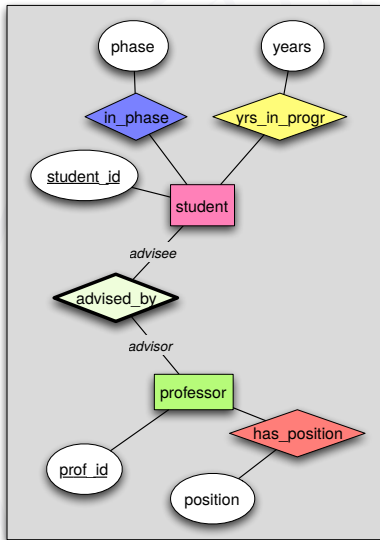
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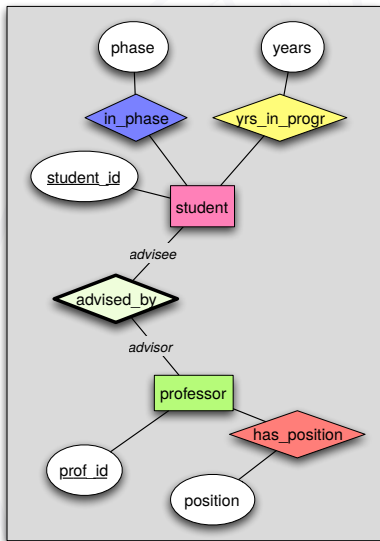
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Similar loss

# kLog by example: UW-CSE

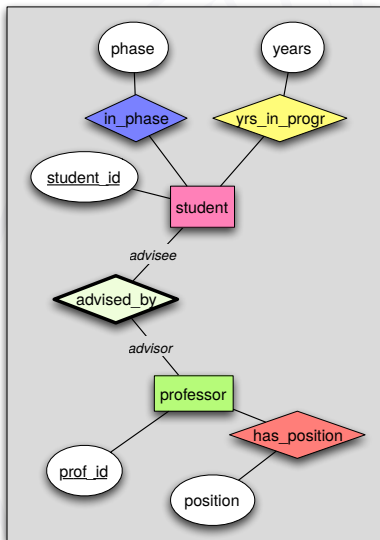


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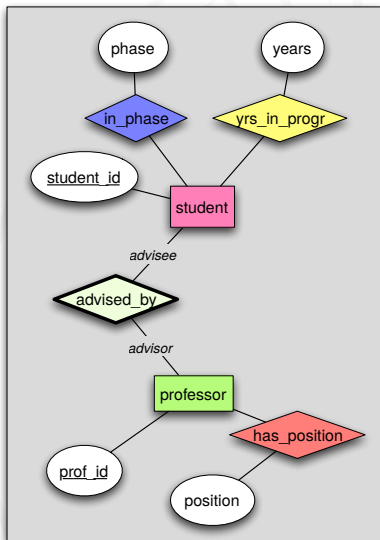
- Classic E/R diagram
- Boxes are **entities**
- Diamonds are **relationships**
- Ovals are **properties**
- Underlined properties are **entity identifiers** (not directly used to create features)

# kLog by example: UW-CSE



```
signature student (  
    student_id::self  
)::extensional.  
signature in_phase (  
    student_id::student,  
    phase::property)::extensional.  
signature years_in_program (  
    student_id::student,  
    years::property  
)::extensional.  
signature professor (  
    prof_id::self  
)::extensional.  
signature has_position (  
    prof_id::professor,  
    position::property  
)::extensional.
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```

- Data is a set of interpretations (in the pure logical sense)
- One interpretation is a set of ground facts

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- In UW-CSE there is one interpretation for every research group (AI, Graphics, etc.)
- Interpretations are *invisible* at the level of kLog scripts (since they are independent, you are not allowed to create interactions)
- The keyword *extensional* declares that all true ground facts for the given predicate are actually given as data (under the usual CWA).

# Example of interpretation

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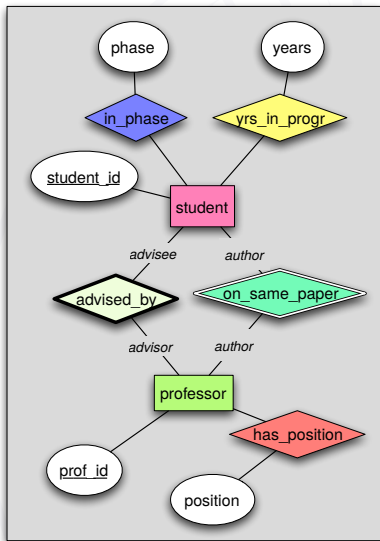
```
interpretation(ai, student(person311)) .
interpretation(ai, student(person14)) .
...
interpretation(ai, professor(person7)) .
interpretation(ai, professor(person185)) .
...
interpretation(ai, has_position(person292, faculty_affiliate)) .
interpretation(ai, has_position(person79, faculty)) .
...
interpretation(ai, in_phase(person139, post_qual)) .
interpretation(ai, in_phase(person333, pre_qual)) .
...
interpretation(ai, years_in_program(person382, year_3)) .
interpretation(ai, years_in_program(person333, year_2)) .
...
interpretation(ai, advised_by(person265, person168)) .
interpretation(ai, advised_by(person352, person415)) .
...
```

# Interpretations may contain more relations

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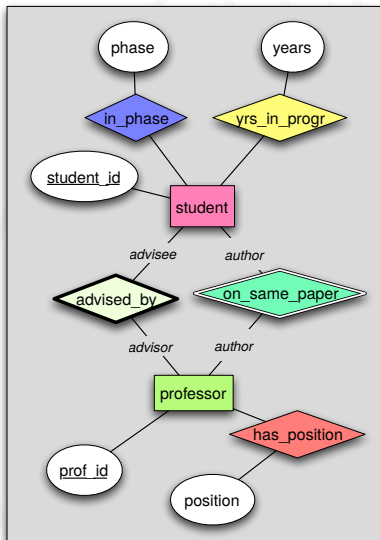
```
interpretation(ai,publication(title25,person284)).
interpretation(ai,publication(title284,person14)).
interpretation(ai,publication(title110,person14)).
...
interpretation(ai,taught_by(course12,person211,autumn_0001)).
interpretation(ai,taught_by(course123,person150,autumn_0001)).
interpretation(ai,taught_by(course44,person293,winter_0001)).
...
interpretation(ai,ta(course44,person193,winter_0304)).
interpretation(ai,ta(course128,person271,winter_0304)).
interpretation(ai,ta(course128,person392,winter_0304)).
```

# Intensional signatures



```
signature on_same_paper(  
  student_id::student,  
  prof_id::professor  
)::intensional.
```

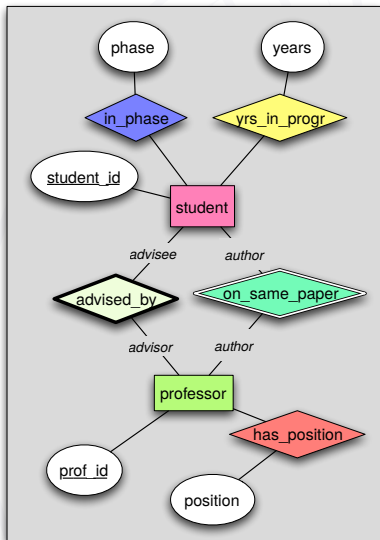
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on_same_paper(S,P) :-  
  student(S), professor(P),  
  publication(Pub, S),  
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```

```
signature on_same_course (  
  student_id::student,  
  prof_id::professor  
)::intensional.
```

```
on_same_course(S,P) :-  
  professor(P), student(S),  
  ta(Course,S,Term),  
  taught_by(Course,P,Term).
```

- Second semantic layer: map each interpretation into a simple graph (not a hypergraph).

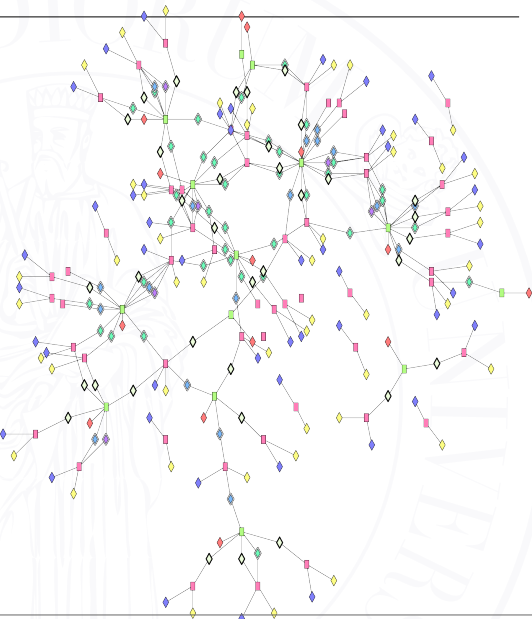
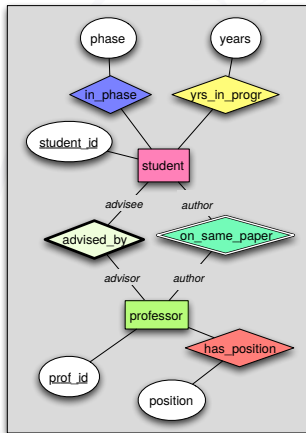
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  - One (undirected) **edge** between  $u$  and  $v$  iff:
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- Graphicalization is essentially grounding the E/R diagram

# Graphicalization in UW-CSE





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- This means to kLog: learn a statistical model capable of predicting tuples for the corresponding relation(s)
- The focus of a job is on **what**, not on **how** (different statistical models can solve the same job – maybe with different performances)

# Single task binary classification

- Job type obtained when we specify a single target signature with **no properties**.

- Example:

```
signature advised_by(  
    s::student,  
    p::professor  
)::extensional.
```

- In this example  $y$  consists of all ground atoms of the relation `advised_by`
- Each tuple of identifiers in the target relation, e.g. a `(student,professor)` pair, is called a **case** (or **instance**)
- if the target signature has entity sets  $\mathcal{E}_1, \dots, \mathcal{E}_k$ , the set of cases is their the Cartesian product



- Single-task multiclass classification: if the target signature contains a categorical property

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- Multi-task: if there are several target signatures or a single target signature with several properties.

# Overview of job types

---

# of properties	Relational arity		
	0	1	2
0	Binary classification of interpretations	Binary classification of entities	Link prediction
1	Multiclass / regression on interpretations	Multiclass / regression on entities	Attributed link prediction
>1	Multitask on interpretations	Multitask predictions on entities	Multitask attributed link prediction

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- In principle any graph kernel can be used and the architecture of kLog is open enough to allow different **feature generators** to be plugged in
- In practice we have implemented a generalization of the Neighborhood Subgraph Pairwise Distance Kernel (NSPDK, Costa & De Grave, ICML 2010)

- Decompose graphs into subgraphs rooted at certain designated vertices called **kernel-points** (KP)
- Consider all pairs of such subgraphs
- Count the number of common pairs between two graphs
- Use hashing to approximate subgraph isomorphism



- Given graph  $G = (V, E)$  and  $u, v \in V$ , let

$$\delta_{u,v} = \begin{cases} \text{SPD}(u, v) & \text{if } u, v \in \text{KP} \\ \infty & \text{otherwise} \end{cases}$$

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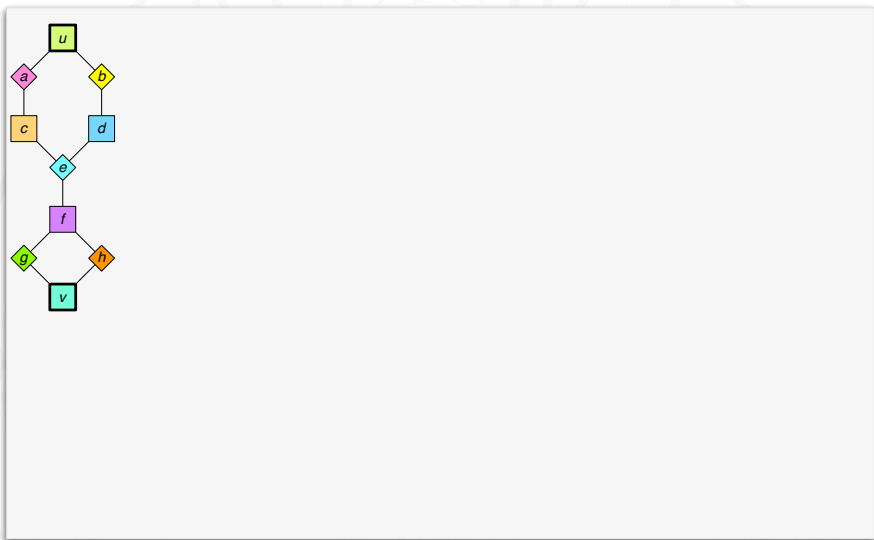
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- The neighborhood-pair (NP) relation is the set of triplets

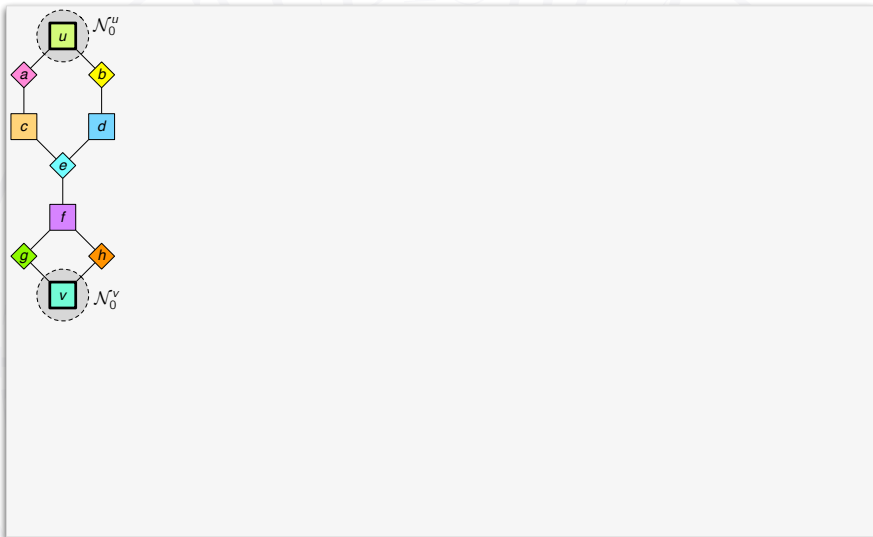
$$R_{r,d} = \{(A, B, G) : A \cong \mathcal{N}_r^v(G), B \cong \mathcal{N}_r^u(G), \delta_{u,v} = d\}$$

where  $\cong$  is graph isomorphism

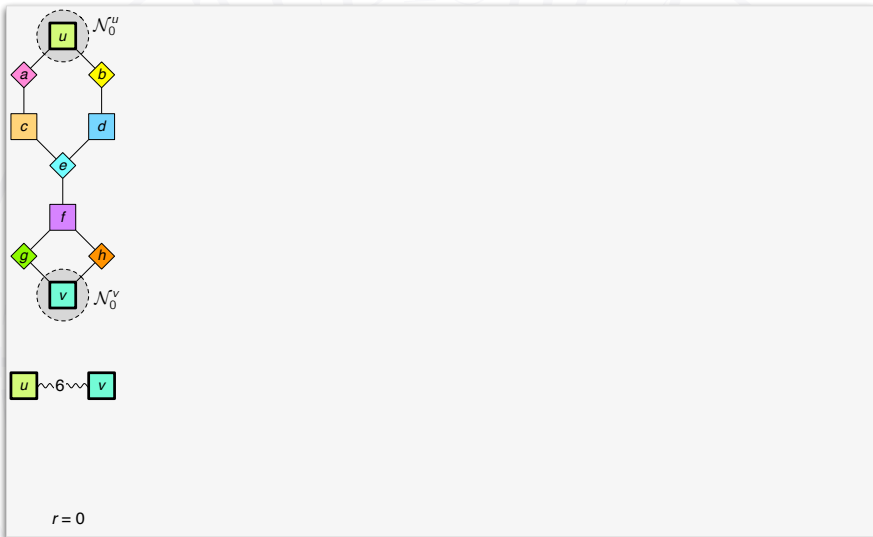
# NP's for fixed $d = 6$



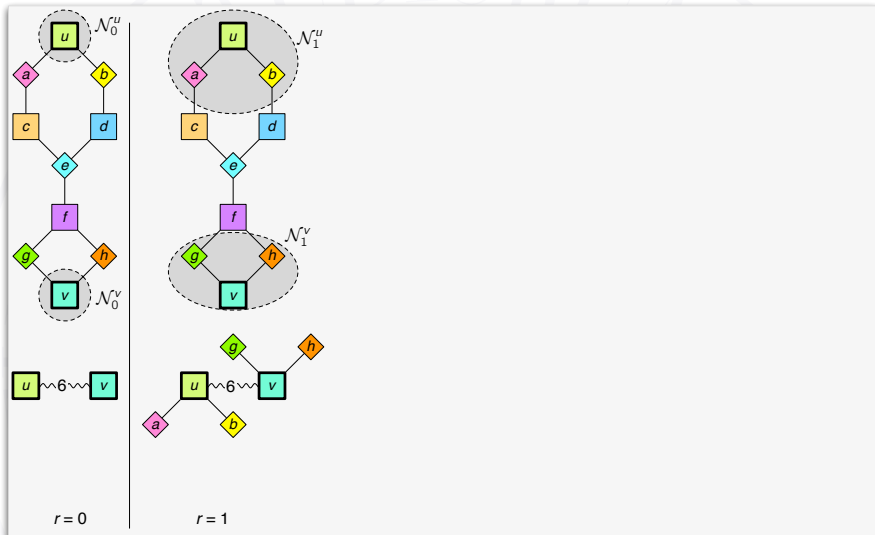
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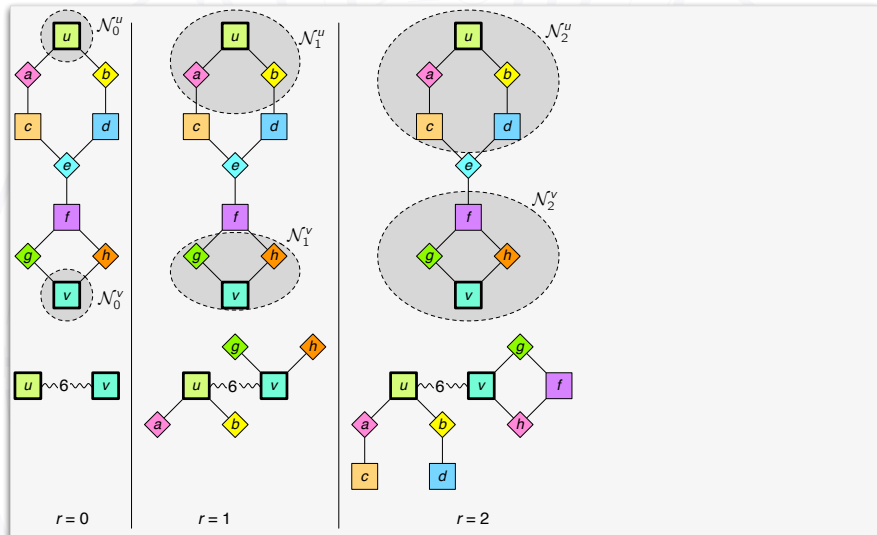
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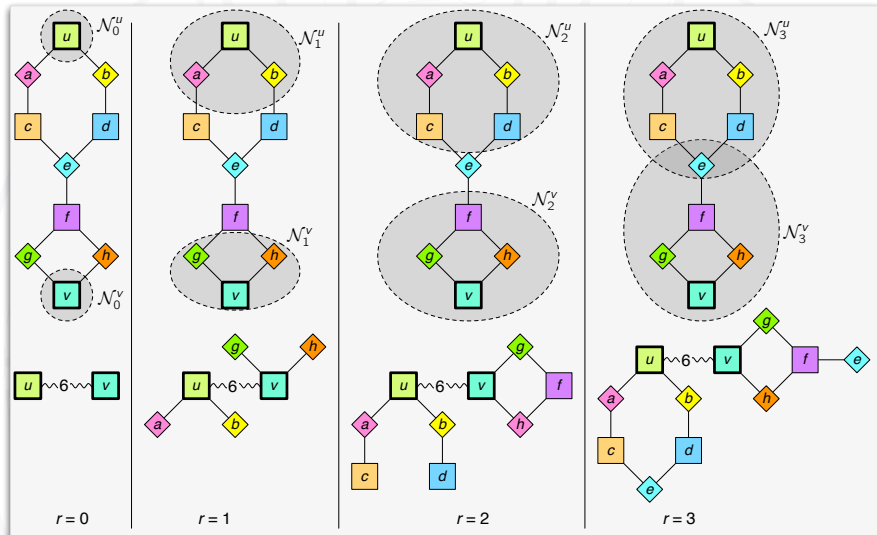


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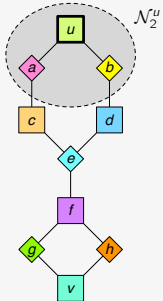




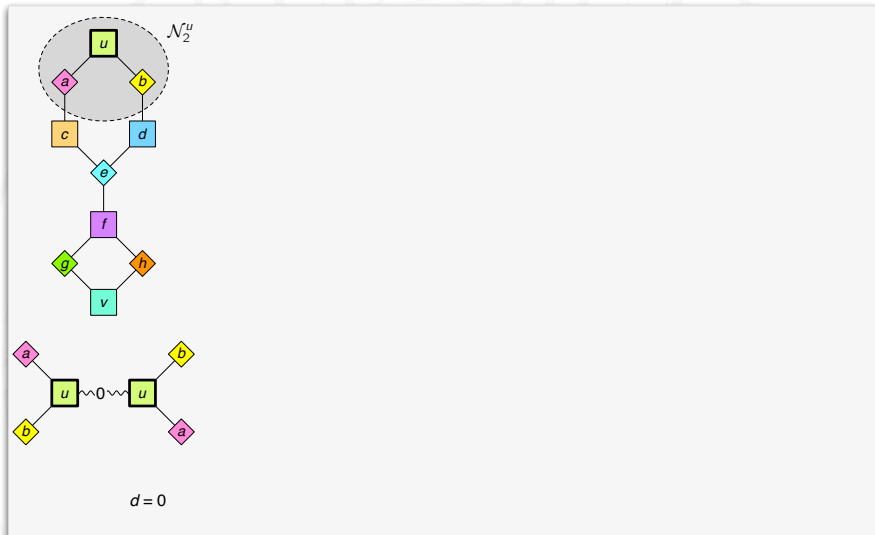
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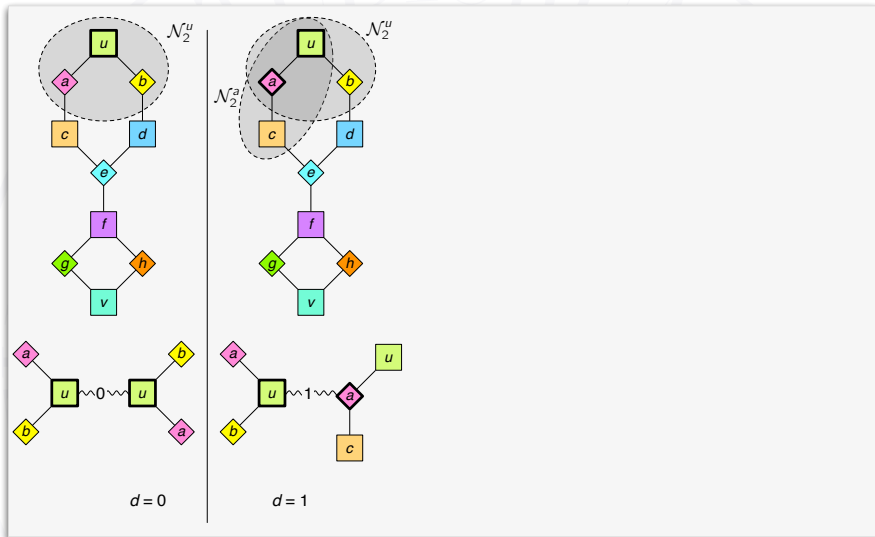
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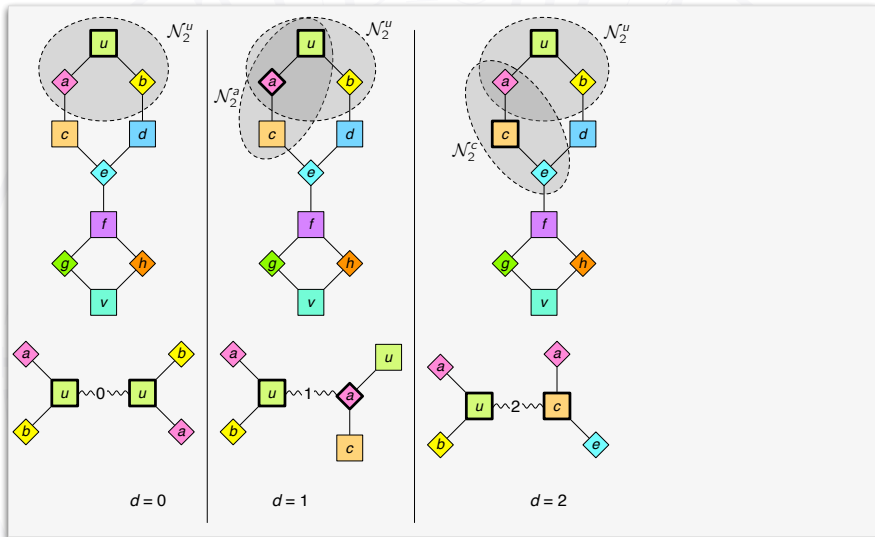
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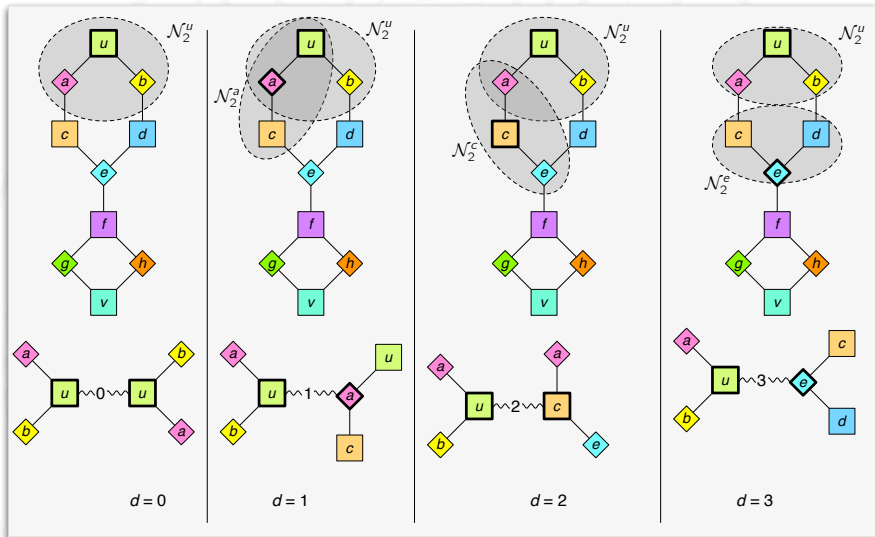
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# Definition of the NSPDK

- $\kappa_{r,d}$  counts common NP's between two graphs:

$$\kappa_{r,d}(G, G') = \sum_{\substack{(A, B) \in R_{r,d}^{-1}(G) \\ (A', B') \in R_{r,d}^{-1}(G')}} \delta(A, A')\delta(B, B')$$

where the “inverse” of a relation  $R \subset \mathcal{A} \times \mathcal{B} \times \mathcal{C}$  is the multiset  $R^{-1}(c) = \{(a, b) : R(a, b, c)\}$

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- Overall kernel:

$$K(G, G') = \sum_{r=0}^R \sum_{d=0}^D \kappa_{r,d}(G, G').$$



- The hard-match might produce very “rare” features depending on the structure of the graph

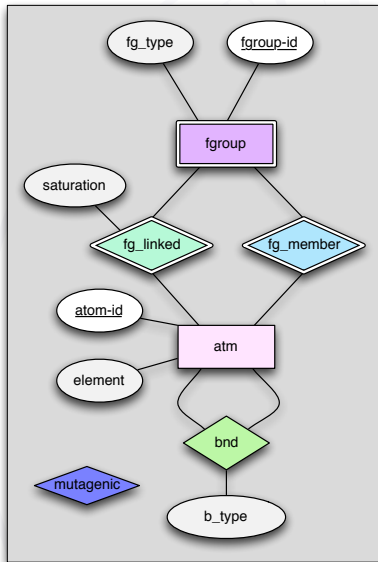
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- Soft match kernel:

$$\kappa_{r,d}(G, G') = \sum_{\substack{(A, B) \in R_{r,d}^{-1}(G) \\ (A', B') \in R_{r,d}^{-1}(G')}} \sum_{v \in V(A) \cup V(B)} \delta(\mathcal{L}(v), \mathcal{L}(v'))$$

where  $\mathcal{L}(v)$  is the label of vertex  $v$

# Example: small molecules



```
signature atm(  
  atom_id::self,  
  element::property)::extensional.
```

```
signature bnd(  
  atom_1@b::atm,  
  atom_1@b::atm,  
  type::property)::extensional.
```

```
signature fgroup(  
  fgroup_id::self,  
  group_type::property  
)::intensional.
```

```
signature fgmember(  
  fg::fgroup,  
  atom::atm)::intensional.
```

```
signature fg_linked(  
  fg::fgroup,  
  alichain::fgroup,  
  saturation::property)::intensional.
```

```
signature mutagenic::extensional.
```

# A whole kLog script

---

```
:- use_module('klog').
begin_domain.
signature atm(atom_id::self,element::property)::extensional.
...
signature activity(act::property)::extensional.
kernel_points([atm,fgroup]).
end_domain.

experiment :-
  new_feature_generator(my_fg,nspdk),
  set_klog_flag(my_fg,radius,4),
  set_klog_flag(my_fg,distance,8),
  attach(bursi_ext),
  new_model(my_model,libsvm_c_svc),
  set_klog_flag(my_model,c,0.5),
  stratified_kfold(mutagenic,10,my_model,my_fg,muta_stratum).
```

# Small molecules (regression/classification)

---

## Biodegradability

Setting	RMSE	SCC	MAPE
Functional groups	$1.07 \pm 0.01$	$0.54 \pm 0.01$	$14.0 \pm 0.1$
Atom bonds	$1.13 \pm 0.01$	$0.48 \pm 0.01$	$14.5 \pm 0.1$

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## Bursi

Setting	AUROC	F1	Error%
Functional groups	$0.91 \pm 0.01$	$86.78 \pm 1.05$	$14.7 \pm 1.5$
Atom bonds	$0.90 \pm 0.01$	$85.21 \pm 1.37$	$16.9 \pm 1.5$

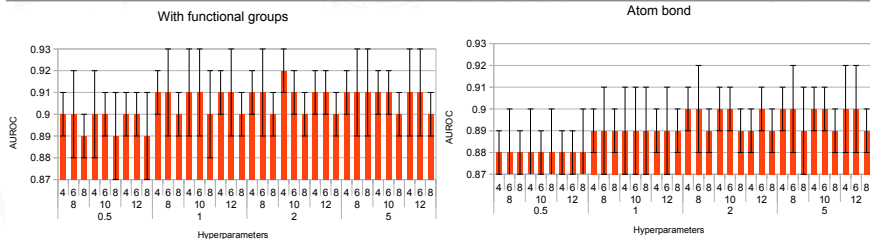
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  - The graph kernel creates joint features  $\phi(x, y)$  so go for **collective** (structured-output) prediction i.e.  $\operatorname{argmax} w' \phi(x, y)$  over an exponential number of assignments to  $y$ . This is especially challenging because intensional predicates need to be re-evaluated for different assignments.

# Is the NPDK kernel general enough?

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  - Project the collective problem into several i.i.d. views

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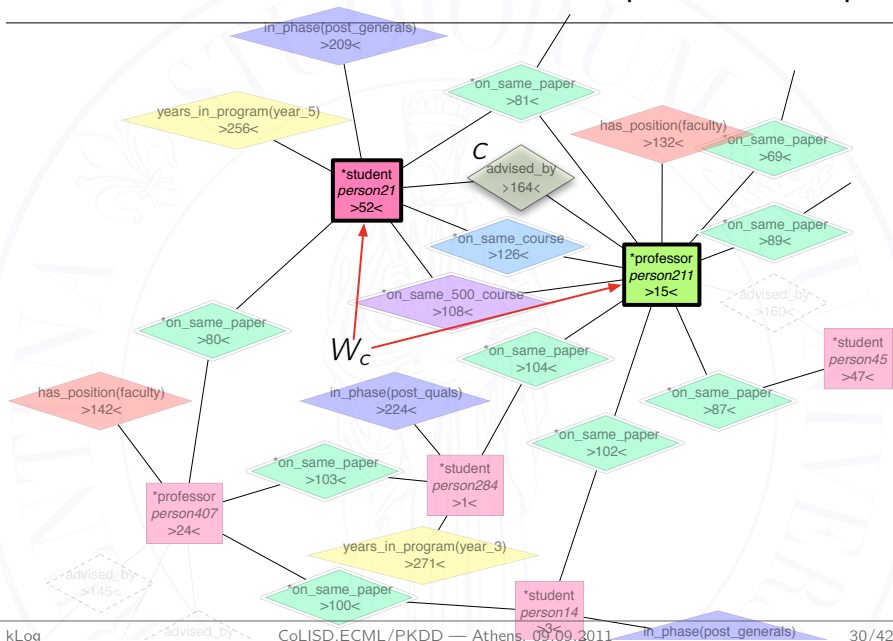
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- Consider the mutilated graph  $G_c$  where all vertices in  $y$  except  $c$  are removed
- Define a kernel  $\hat{\kappa}$  on mutilated graphs: like NSPDK but with the restriction that the first endpoint must be in  $W_c$

$$\hat{R}_{r,d} = \{(A, B, G_c) : A \cong \mathcal{N}_r^v, B \cong \mathcal{N}_r^u, v \in W_c, \delta_{u,v} = d\}$$



# Viewpoints example



# View points and i.i.d. views (non-collective)

- We get in this way a kernel “centered” around case  $c$ :

$$\hat{K}(G_c, G'_c) = \sum_{r,d} \sum_{\substack{A, B \in \hat{R}_{r,d}^{-1}(G_c) \\ A', B' \in \hat{R}_{r,d}^{-1}(G'_c)}} \delta(A, A') \delta(B, B')$$

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- Finally let

$$K(G, G') = \sum_{c \in \mathcal{Y}, c' \in \mathcal{Y}'} \hat{K}(G_c, G'_{c'})$$

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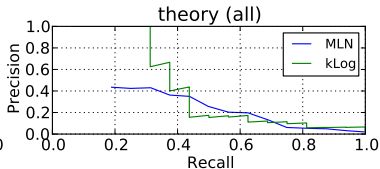
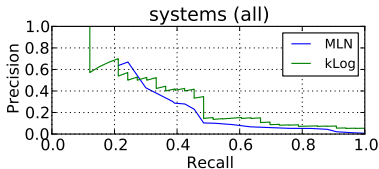
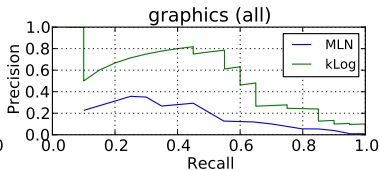
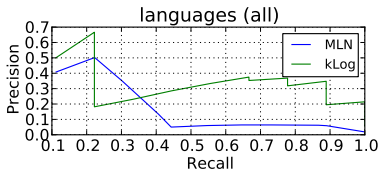
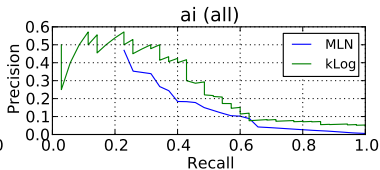
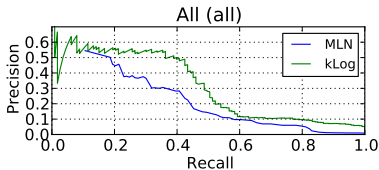
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- This kernel corresponds to the potential

$$F(x, y) = w' \sum_c \hat{\phi}(x, c)$$

which is clearly maximized by maximizing, independently, all sub-potentials  $w' \hat{\phi}(x, c)$  with respect to  $c$ .



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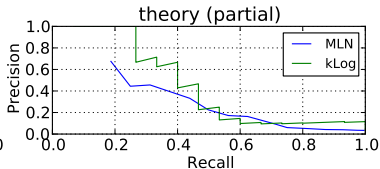
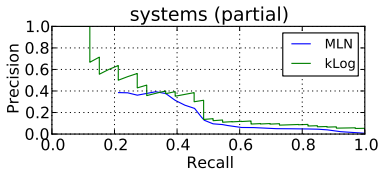
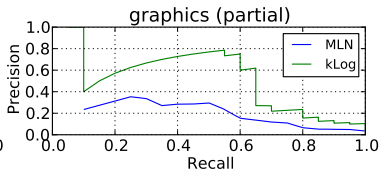
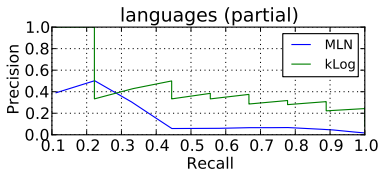
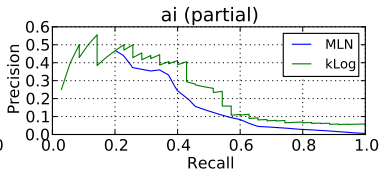
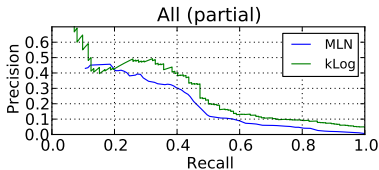


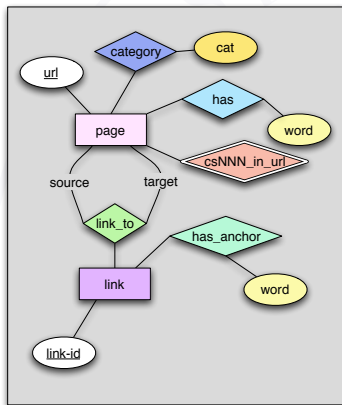
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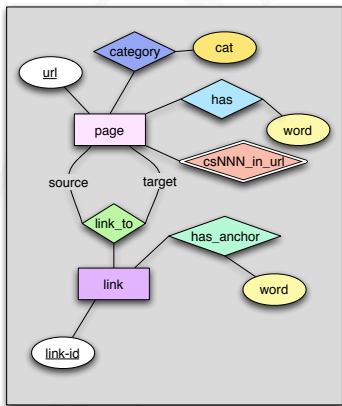
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  - Learn the binary relation taking saved groundings as additional data

# UW-CSE: Partial information







```

...
signature csNNN_in_url(
    pageid::page
)::intensional.

csNNN_in_url(Url) :-
    page(Url),
    atom_codes(Url,CUrl),
    regexp("cs(e*)[0-9]+",CUrl,[],[_Match]).

signature category(
    page_id::page,
    cat::property
)::extensional.

...

```

# Cases: 1039

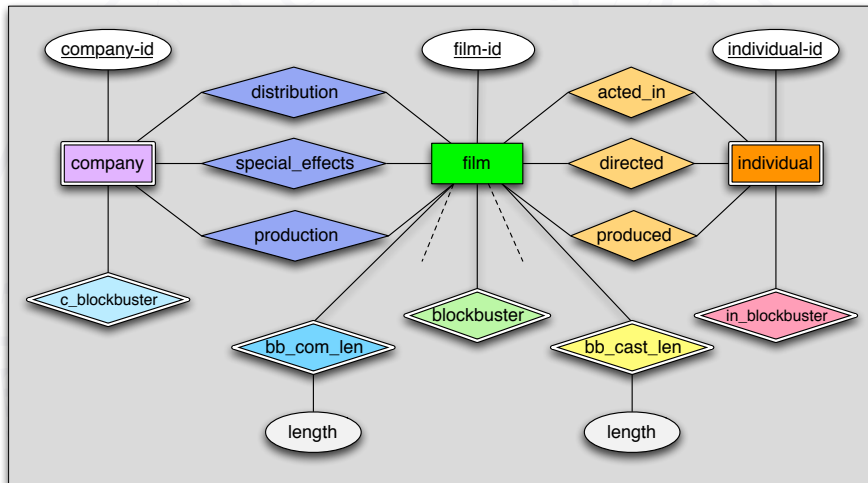
Case error rate: 12.42%

Interpretation error rate: 100.00%

Contingency table: (rows are predictions)

	researc	faculty	course	student	
researc	59	11	4	15	a,p,r,f1= 0.94 0.66 0.70 0.68
faculty	9	125	2	50	a,p,r,f1= 0.91 0.67 0.82 0.74
course	0	0	233	0	a,p,r,f1= 0.99 1.00 0.95 0.98
student	16	17	5	493	a,p,r,f1= 0.90 0.93 0.88 0.91
Average p,r,f1 =	0.89	0.88	0.88		

# Internet Movies Database





---

signature **blockbuster**(*film\_id::film*)::intensional.

blockbuster(M) :-

opening\_weekend(M,Receipts),

Receipts > 2000000.

---

```
signature blockbuster(film_id::film)::intensional.
blockbuster(M) :-
    opening_weekend(M,Receipts),
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signature individual(individual_id::self)::intensional.
individual(P) :-
    person(P,_Name), active_enough(P).
has_active_role(P,M) :- acted_in(P,M).
has_active_role(P,M) :- directed(P,M).
has_active_role(P,M) :- produced(P,M).
active_enough(P) :-
    setof(M,has_active_role(P,M),Ms), length(Ms,N), N>2.
```

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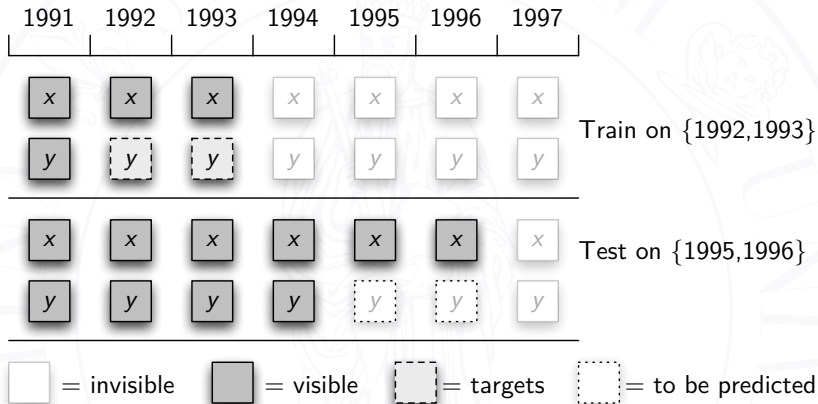
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active_enough(P) :-
    setof(M,has_active_role(P,M),Ms), length(Ms,N), N>2.

signature in_blockbuster(individual_id::individual)::intensional.
in_blockbuster(P) :-
    has_active_role(P,M),
    blockbuster(M).

signature bb_cast_len(film_id::film,n::property)::intensional.
bb_cast_len(M,N) :-
    setof(Actor,(acted_in(Actor,M), in_blockbuster(Actor)), Set),
    length(Set,N).
```

- In a data set like IMDb there is one single interpretation
- How to split training and test data?

# Slicing



## IMDb: results

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Year	movies	facts	AUROC
1995	74	2483	-
1996	223	6406	-
1997	311	8031	0.85
1998	332	7822	0.92
1999	348	7842	0.88
2000	381	8531	0.95
2001	363	8443	0.94
2002	370	8691	0.93
2003	343	7626	0.94
2004	371	8850	0.94
2005	388	9093	0.92
All			0.92 $\pm$ 0.03

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## ■ Applications (work in progress)

- Information extraction from text, e.g. spatial role labeling (Kordjamshidi et al. 2011)
- Hedge cue detection, e.g. recognition of weasel sentences (Verbeke et al. 2011)
- Vision, e.g. image segmentation/labeling (Antanas et al. 2011)