

# Declarative Modeling for Machine Learning and Data Mining

*Lab for Declarative Languages and Artificial Intelligence*

*Joint work with especially  
Tias Guns and Siegfried Nijssen and Paolo Frasconi  
and the EU FET ICON project*

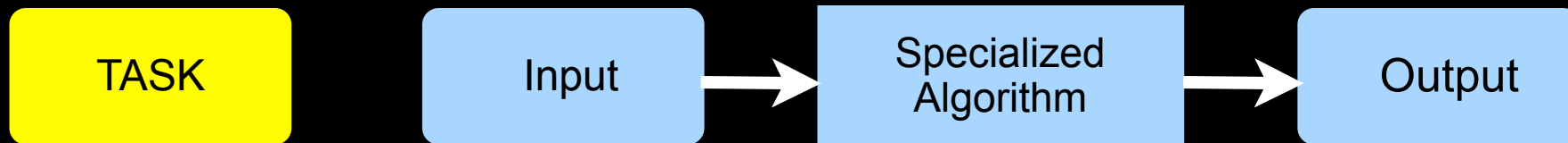
**KU LEUVEN**

(c) Luc De Raedt

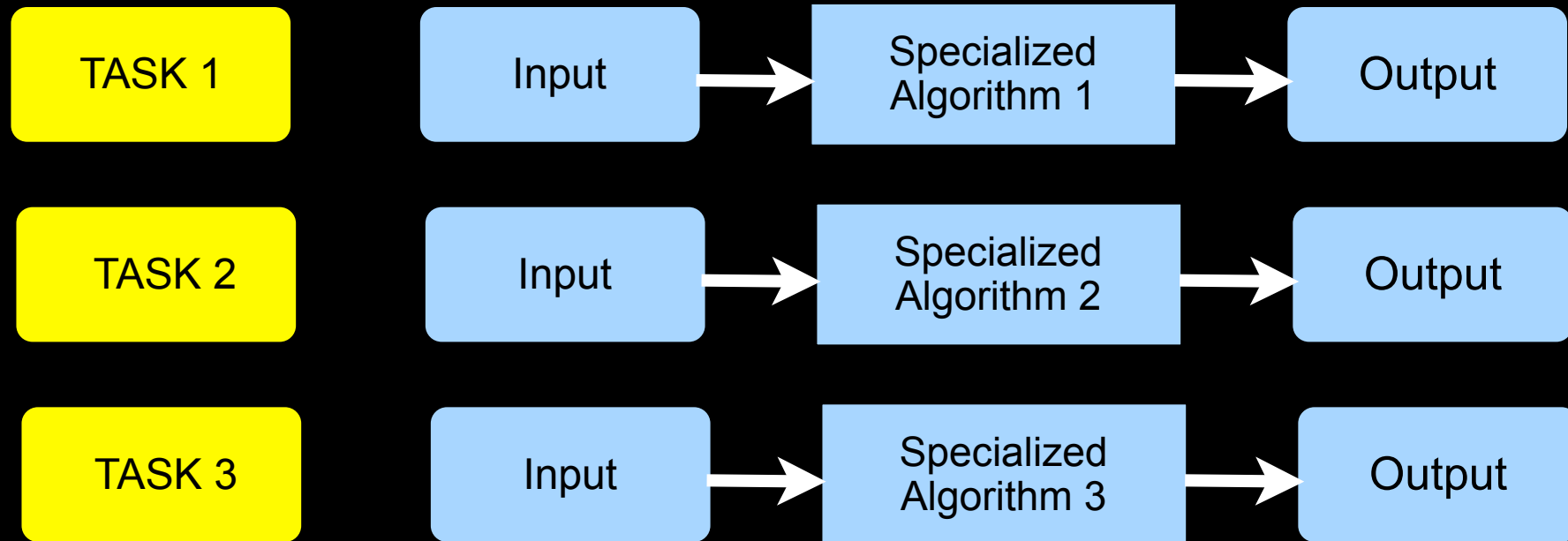
# Our work today ...

We typically ...

1. Formalize learning / mining task
2. Design algorithm / technique to use
3. Implement the algorithm
4. Use and distribute the software



# And do it again ...



# Our work today ...

We typically ...

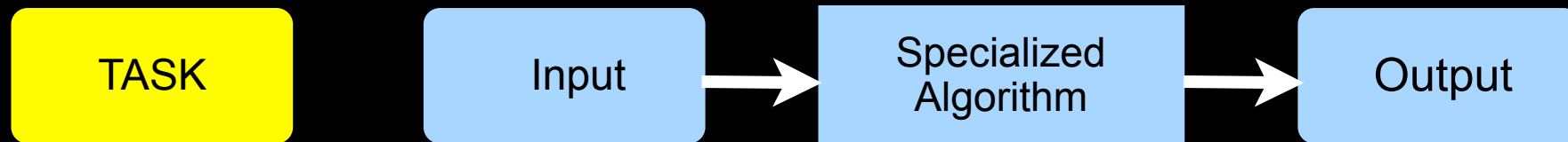
1. Formalize learning / mining task

2. Design algorithm / technique to use

hard

3. Implement the algorithm

4. Use and distribute the software



# The Challenge

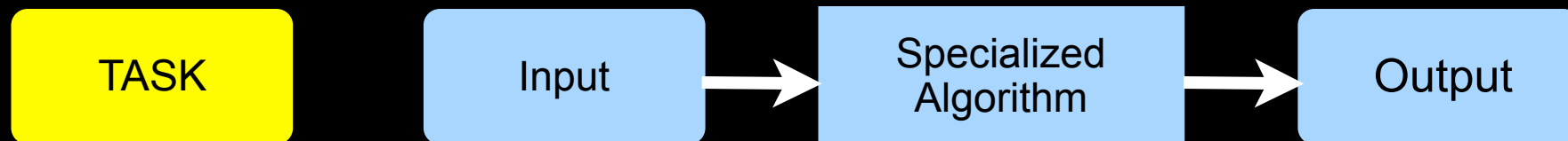
Cannot we simplify this ... ?

1. Formalize learning / mining task

~~2. Design algorithm / technique to use~~

~~3. Implement the algorithm~~

4. Use and distribute the software



# Key Point

The key point I want to make is that  
**POTENTIALLY we can** by adopting a  
**Declarative Modeling paradigm**

first steps have been taken ...  
e.g. use of **Convex Optimisation**

# Overview Talk

- The Challenge:
  - from Programming to Modeling for ML/DM
- The what, why and how of Declarative Modeling (and Constraint Programming)
- How does this relate to ML/DM ?
- Evidence: a case study in pattern mining
- Perspective / Discussion

The What, Why and How  
of  
Declarative Modeling



# What is declarative modeling ?

Model

```
array [1..9, 1..9] of var 1..9: sq;  
predicate row_diff(int: r) =  
    all_different (c in 1..9) (sq[r, c]);  
predicate col_diff(int: c) =  
    all_different (r in 1..9) (sq[r, c]);  
predicate subgrid_diff(int: r, int: c) =  
    all_different (i, j in 0..2) (sq[r + i, c + j]);  
  
constraint forall (r in 1..9) (row_diff(r));  
constraint forall (c in 1..9) (col_diff(c));  
constraint forall (r, c in {1, 4, 7}) (subgrid_diff(r, c))  
  
solve satisfy;
```

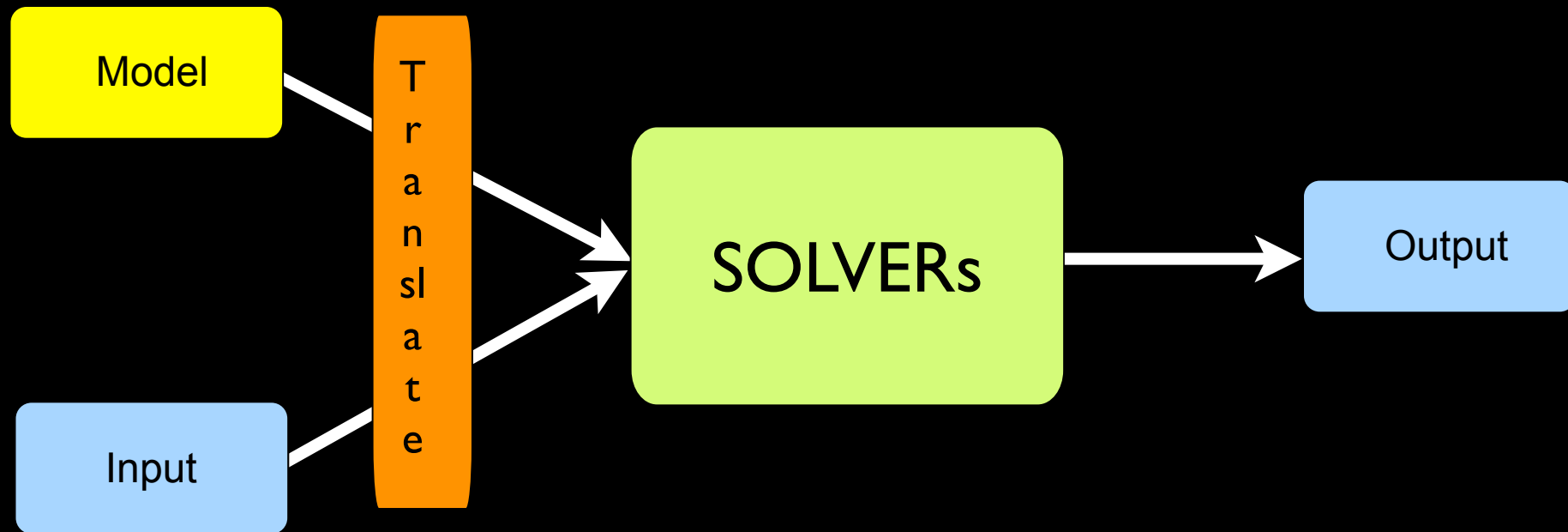
Inputs

1								6
		6		2		7		
7	8	9	4	5		1		3
			8		7			4
				3				
	9				4	2		1
3	1	2	9	7			4	
	4			1	2		7	8
9		8						

Zinc family of languages

# How does it work ?

MODEL specifies task = constraints  
+ optimization criterion



Data = Input

state WHAT the problem is  
different SOLVERs possible

# Why declarative modeling ?

## DECLARATIVE

- few lines of code
- easy to understand, maintain, change
- can be used with multiple “solvers”, e.g., exact and approximate
- formal verification possible

## PROCEDURAL

- 1000s of lines of code
- hard to understand, maintain or change
- solver is built in the program

Here - CONSTRAINT PROGRAMMING  
Also -- ANSWER SET PROGRAMMING

# Constraint Programming

## Given

- a set of variables  $V$
- the domain  $D(x)$  of all variables  $x$  in  $V$
- a set of constraints  $C$  on values these variables can take

CSP

**Find** an assignment of values to variables in  $V$  that satisfies all constraints in  $C$

Zinc [Garcia de la Banda *et al.* CP 06]

# Constraint Satisfaction

Person



P1



P2



P3



P4

Office

1



2



Solutions



2



1



2



1



```
var P1, P2, P3, P4: {1,2};
```

```
constraint P1 != P2;
```

```
constraint P3 != P4;
```

```
constraint P1 != 1;
```

```
solve satisfy;
```

# Solvers for CP

## Two key ideas

- propagation of constraints, e.g., from

*$D(P1) = \{1\}$  and  $D(P2) = \{1,2,3\}$  and  $P1 \neq P2$  infer that  $1 \notin D(P2)$  and simplify  $D(P2) = \{2,3\}$*

***propagator:** if  $D(x) = \{d\}$  and  $x \neq y$  then delete  $d$  from  $D(y)$*

- if you cannot propagate, instantiate (or divide) and recurse, e.g.,

*call with  $D(P2)=\{2\}$       and      with  $D(P2)=\{3\}$*

*$P2=2$*

*$P2=3$*

Person

Office



P1



P2



P3



P4

1



2

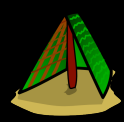


Solutions



2

1



2

1

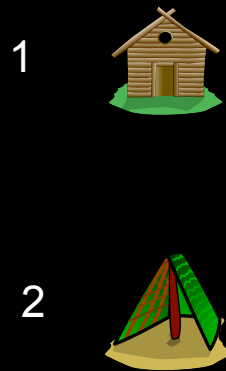


# Search

Person



Office

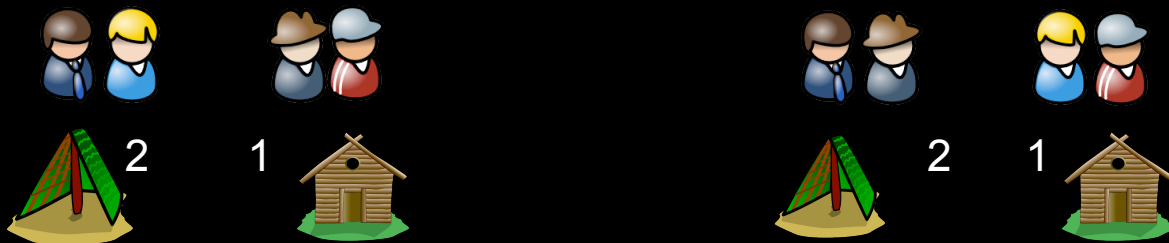


$$\begin{aligned} D(P1) &= \{1,2\} \\ D(P2) &= \{1,2\} \\ D(P3) &= \{1,2\} \\ D(P4) &= \{1,2\} \end{aligned}$$

$$P1 \neq P2$$

$$P3 \neq P4$$

Solutions



$$P1 \neq 1$$



# Search

Person



P1



P2



P3



P4

Office

1



2



Solutions



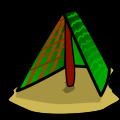
2



1



2



1



$$D(P1) = \{1,2\}$$

$$D(P2) = \{1,2\}$$

$$D(P3) = \{1,2\}$$

$$D(P4) = \{1,2\}$$

$$P1 \neq P2$$

$$P3 \neq P4$$

$$P1 \neq 1$$

# Search

Person



P1



P2



P3



P4

Office

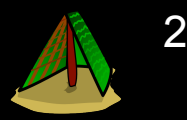
1



2



Solutions



$$D(P1) = \{ 2 \}$$

$$D(P2) = \{ 1, 2 \}$$

$$D(P3) = \{ 1, 2 \}$$

$$D(P4) = \{ 1, 2 \}$$

$$P1 \neq P2$$

$$P3 \neq P4$$

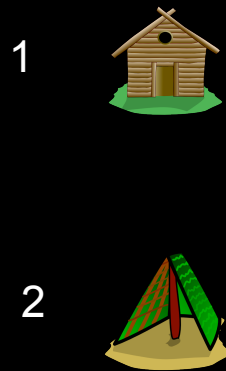
$$P1 \neq 1$$

# Search

Person



Office



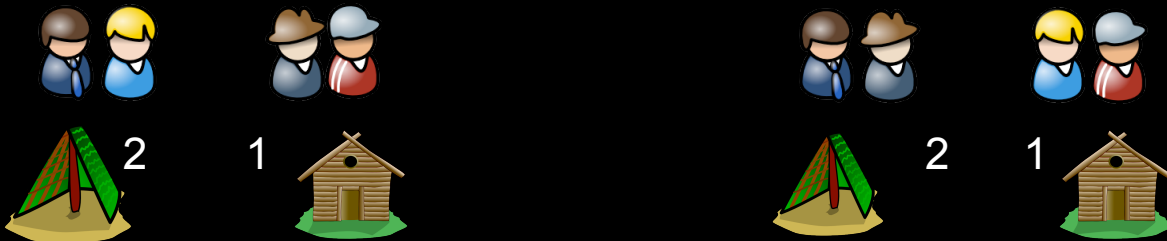
$$\begin{aligned} D(P1) &= \{ 2 \} \\ D(P2) &= \{ 1, 2 \} \\ D(P3) &= \{ 1, 2 \} \\ D(P4) &= \{ 1, 2 \} \end{aligned}$$

$$P1 \neq P2$$

$$P3 \neq P4$$

$$P1 \neq 1$$

Solutions



# Search

Person



P1



P2



P3



P4

Office

1



2



Solutions



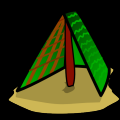
2



1



2



1



choose P3 = 1

$$D(P1) = \{ 2 \}$$

$$D(P2) = \{ 1 \}$$

$$D(P3) = \{ 1, 2 \}$$

$$D(P4) = \{ 1, 2 \}$$

$$P1 \neq P2$$

$$P3 \neq P4$$

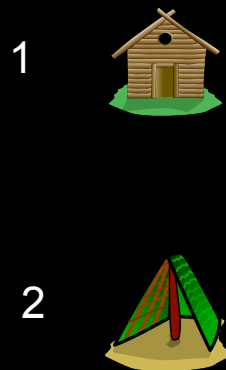
$$P1 \neq 1$$

# Search

Person



Office

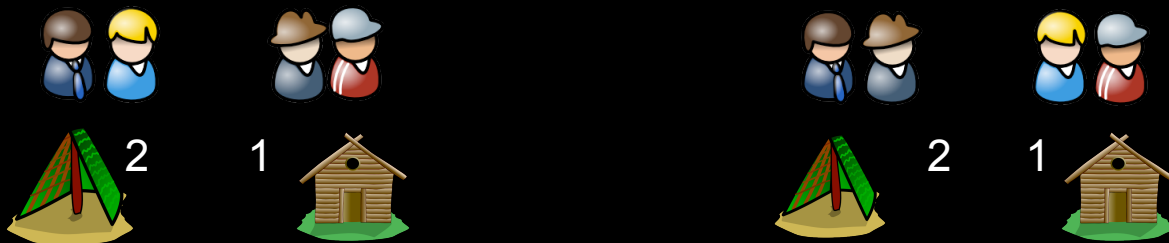


$$D(P1) = \{ 2 \}$$
$$D(P2) = \{ 1 \}$$
$$D(P3) = \{ 1 \}$$
$$D(P4) = \{ 1, 2 \}$$

$$P1 \neq P2$$

$$P3 \neq P4$$

Solutions



$$P1 \neq 1$$

# Search

Person



P1



P2



P3



P4

Office

1



2



Solutions



2



1



2



1



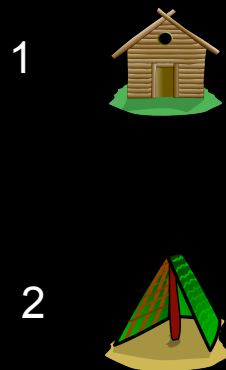
& backtrack

# Search

Person



Office



$$D(P1) = \{ 2 \}$$
$$D(P2) = \{ 1 \}$$
$$D(P3) = \{ 1, 2 \}$$
$$D(P4) = \{ 1, 2 \}$$

$$P1 \neq P2$$

$$P3 \neq P4$$

$$P1 \neq 1$$

Solutions



# Search

Person



P1



P2



P3



P4

Office

1



2



Solutions



2



1



2



1



$$D(P1) = \{ 2 \}$$

$$D(P2) = \{ 1 \}$$

$$D(P3) = \{ 2 \}$$

$$D(P4) = \{ 1, 2 \}$$

$$P1 \neq P2$$

$$P3 \neq P4$$

$$P1 \neq 1$$

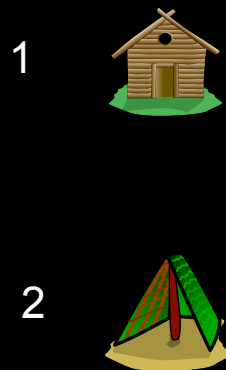


# Search

Person



Office

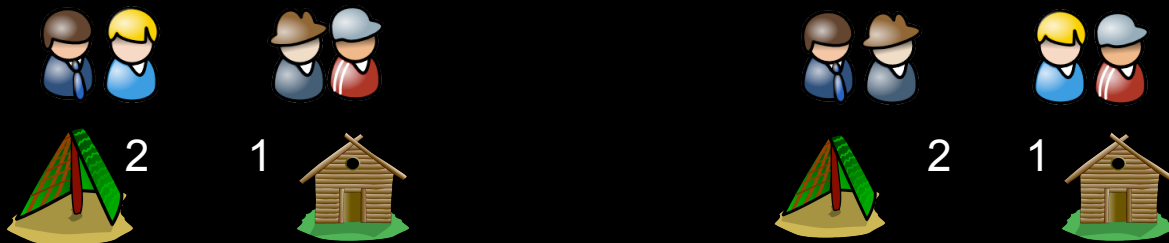


$$\begin{aligned} D(P1) &= \{ 2 \} \\ D(P2) &= \{ 1 \} \\ D(P3) &= \{ 2 \} \\ D(P4) &= \{ 1 \} \end{aligned}$$

$$P1 \neq P2$$

$$P3 \neq P4$$

Solutions



$$P1 \neq 1$$

# Constraint Programming

There is a lot more to say

- about types of constraints and domains used
- about modeling languages
- about propagators -- how to modify domains
- about choosing the next variable to instantiate
- about implementations ...
- about their **incorporation in programming languages ...**
- about their **performance ...**

What about ML/DM ?

# Observation I

Machine learning and data mining are essentially constraint satisfaction and optimization problems

# Data Mining

## Given

- a database containing instances or transactions  $D$   
the set of instances
- a hypothesis space or pattern language  $L$
- a selection predicate, query or set of constraints  $Q$

**Find**  $Th(Q,L,D) = \{ h \in L \mid Q(h,D) = \text{true} \}$

[Mannila and Toivonen, 96]

# Itemset mining

## Given

- a set of items  $I$
- a transaction  $t \subseteq I$ . So,  $X = 2^I$
- $D$  is a set of transactions.
- $L = X = 2^I$
- a frequency threshold  $c$ , with  $\text{freq}(h,D) = |\{d \mid d \in D, h \subseteq d\}|$

**Find**  $\text{Th}(Q,L,D) = \{h \in L \mid \text{freq}(h,D) > c\}$

# Machine learning

## Given

- an unknown target function  $f: X \rightarrow Y$
- a hypothesis space  $L$  containing functions  $X \rightarrow Y$
- a dataset of examples  $E = \{ (x, f(x)) \mid x \in X \}$
- a loss function  $loss(h, E) \rightarrow \mathbb{R}$

**Find**  $h \in L$  that minimizes  $loss(h, E)$

supervised



# Observation I

Machine learning and data mining are essentially  
constraint satisfaction and optimization  
problems

well-known in ML and DM  
good news



# Observation 2

Use of solvers is very common in  
statistical learning (and SVMs)

- convex optimization and mathematical programming solvers

graphical models

- knowledge compilation packages and belief propagation

**An important factor for their success**

# Observation 2

There has been a paradigm shift in the field of AI from **programming** to **solving** (Hector Geffner at ECAI 2012)

Today AI uses **solvers** for crisp computational problems

- SAT, ASP, CSP, CP, maxSAT, weighted model counting, ...
- many problems are reduced to these basic problems ... and solved efficiently

**Still less common in other areas of DM/ML**

# Observation 3

There has been an enormous progress in solver technology for basic constraint satisfaction and optimization problems

Solver technology facilitates the development of high-level declarative modeling languages

- specify the **WHAT** -- not the **HOW**

Examples include

- ZINC, Essence, Comet, OPL, FO(.), ...

Very flexible approach ...

**Still less common in DM/ML (except Matlab ?)**

# Long standing open questions

Tom Mitchell, *The Discipline of Machine Learning*, 2006

Can we design programming languages containing machine learning primitives?

Can a new generation of computer programming languages directly support writing programs that learn?

... some subroutines are hand-coded while others are **specified** as “to be learned.” ... the programmer **declares** the **inputs and outputs** of each “to be learned” subroutine, **then selects a learning algorithm** ...

# Questions remain open

Though relevant work on

- probabilistic & adaptive programming languages
- inductive query languages for data mining [Imielinski and Mannila, 95; EU clnQ and IQ projects]
- inductive logic programming and statistical relational learning
- Learning based Java [Roth et al. 10] and kLog [Frasconi et al.]

Can we obtain programming languages for ML / DM  
by applying the principles of constraint programming ?

Evidence

The case of Pattern mining

# Pattern Mining

## A. frequent pattern

- which patterns are frequent ?

$$Th(\mathcal{L}, Q, \mathcal{D}) = \{p \in \mathcal{L} \mid Q(p, \mathcal{D}) = true\}$$

## B. Correlated pattern mining = subgroup discovery

- which patterns are significant w.r.t. classes ? all patterns ? k-best patterns ?

$$Th(\mathcal{L}, Q, \mathcal{D}) = \arg_{p \in \mathcal{L}} \max_k \phi(p, \mathcal{D})$$

## C. pattern set mining

- which pattern set is the *best* concept-description for the actives ? for the inactives ?

$$Th(\mathcal{L}, Q, \mathcal{D}) = \{P \subseteq \mathcal{L} \mid Q(P, \mathcal{D}) = true\}$$

# Pattern Mining

## A. frequent pattern

- which patterns are frequent ?

$$Th(\mathcal{L}, Q, \mathcal{D}) = \{P \subseteq \mathcal{L} \mid Q(P, \mathcal{D}) = true\}$$

## B. Correlated pattern

- which patterns are correlated ?

Part

We have been using off-the-shelf CP SOLVERS for these tasks, cf. Guns, Nijssen, De Raedt [AAAI 10, AIJ 11]

One solver for all of these

Easy to combine different constraints

Now looking at modeling level

KDD 08

KDD 09

## C. pattern

- which patterns are concept-descriptions for the actives ?  
for the

IEEETKDE 11

$$Th(\mathcal{L}, Q, \mathcal{D}) = \{P \subseteq \mathcal{L} \mid Q(P, \mathcal{D}) = true\}$$

$$\phi(p, \mathcal{D})$$



# A. Frequent Pattern Mining

# A. Frequent Itemset Mining

Given

- $\mathcal{I} = \{1, \dots, NrI\}$   
set of items
- $\mathcal{T} = \{1, \dots, NrT\}$   
set of transactions identifiers
- $\mathcal{D} = \{(t, I) | t \in \mathcal{T}, I \subseteq \mathcal{I}\}$   
Dataset
- $Items \subseteq \mathcal{I}$  and  $Trans \subseteq \mathcal{T}$

Find *Items* such that

$$|covers(Items, \mathcal{D})| > freq$$

where  $covers(Items, \mathcal{D}) =$   
 $\{t \in \mathcal{T} | (t, I) \in \mathcal{D} \text{ and } Items \subseteq I\}$

# A. Frequent Itemset Mining

Given

- $\mathcal{I} = \{1, \dots, NrI\}$   
set of items
- $\mathcal{T} = \{1, \dots, NrT\}$   
set of transactions identifiers
- $\mathcal{D} = \{(t, I) | t \in \mathcal{T}, I \subseteq \mathcal{I}\}$   
Dataset
- $Items \subseteq \mathcal{I}$  and  $Trans \subseteq \mathcal{T}$

Find  $Items$  such that  
 $|covers(Items, \mathcal{D})| > freq$

where  $covers(Items, \mathcal{D}) =$   
 $\{t \in \mathcal{T} | (t, I) \in \mathcal{D} \text{ and } Items \subseteq I\}$

```
int: Freq;  
int: NrI;  
int: NrT;
```

```
array[1..NrT] of set of 1..NrI: D;
```

```
var set of 1..NrI: Items;  
var set of 1..NrT: Trans;
```

```
constraint card(Trans) > Freq;  
constraint Trans = covers(Items, D);
```

```
solve satisfy;
```

```
function var set of int: cover(Items, D) =  
let {  
    var set of int: Trans,  
    constraint forall (t in ub(Trans))  
        (t in Trans  $\leftrightarrow$  Items subset D[t])  
} in Trans;
```

# Frequent Itemset Mining

math like notation

user defined functions and  
constraints

solver independent  
(standardized)

efficiently solvable

```
int: Freq;  
int: NrI;  
int: NrT;
```

```
array[1..NrT] of set of 1..NrI: D;
```

```
var set of 1..NrI: Items;  
var set of 1..NrT: Trans;
```

```
constraint card(Trans) > Freq;  
constraint Trans = covers(Items, D);
```

```
solve satisfy;
```

```
function var set of int: cover(Items, D) =  
let {  
    var set of int: Trans,  
    constraint forall (t in ub(Trans))  
        (t in Trans  $\leftrightarrow$  Items subset D[t])  
} in Trans;
```

# Closed Itemset Mining

```
function var set of int: cover_inv(Trans,D)=  
let {  
    var set of int: Items,  
    constraint forall (i in ub(Items))  
        (i in Items  $\leftrightarrow$  Trans subset D'[i] )  
} in Items;
```

```
function var set of int: cover(Items, D) =  
let {  
    var set of int: Trans,  
    constraint forall (t in ub(Trans))  
        (t in Trans  $\leftrightarrow$  Items subset D[t] )  
} in Trans;
```

```
int: Freq;  
int: NrI;  
int: NrT;
```

```
array[1..NrT] of set of 1..NrI: D;
```

```
var set of 1..NrI: Items;  
var set of 1..NrT: Trans;
```

```
constraint card(Trans) > Freq;  
constraint Trans = covers(Items, D);  
constraint Items = cover_inv(Trans, D);  
solve satisfy;
```

# Further Constraints

\* exact coverage :

$t \text{ in Trans} \leftrightarrow \text{Items} \text{ subset } D[t]$

\* freq:

$i \text{ in Items} \rightarrow \text{card}(\text{Trans} \text{ intersect } D'[i]) \geq \text{Freq}$

\* maximal:

$i \text{ in Items} \leftrightarrow \text{card}(\text{Trans} \text{ intersect } D'[i]) \geq \text{Freq}$

\* closed:

$i \text{ in Items} \leftrightarrow \text{Trans} \text{ subset } D'[i]$

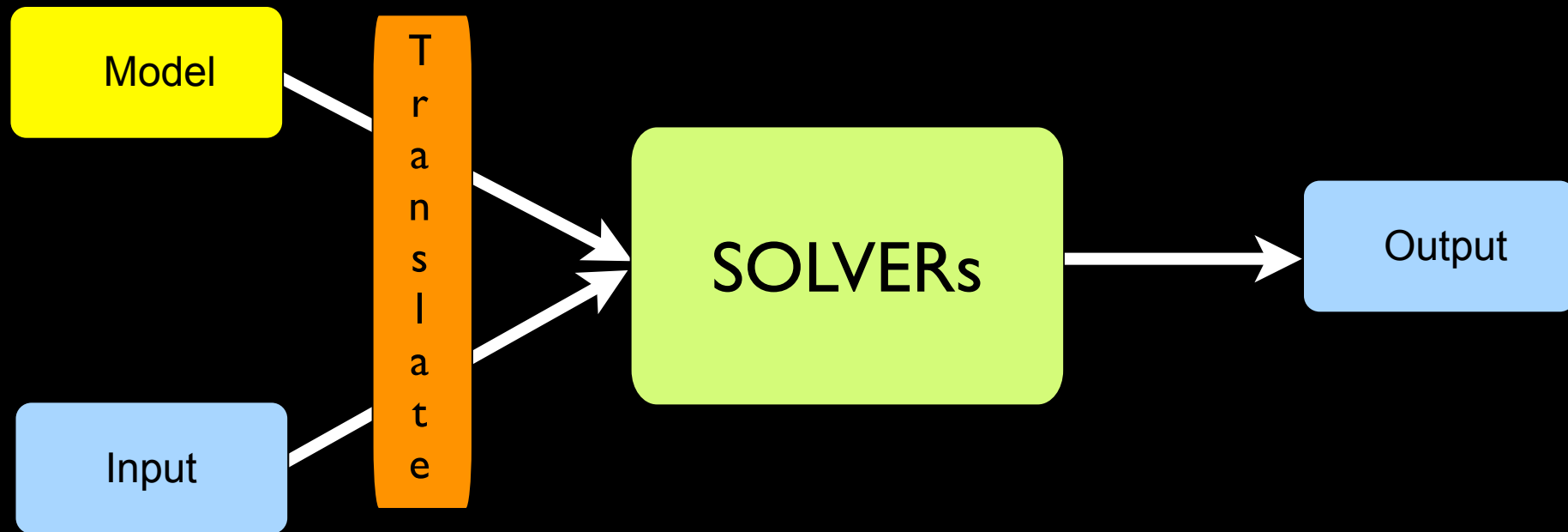
\* delta-closed:

$i \text{ in Items} \leftrightarrow \text{card}(\text{Trans} \text{ intersect } D'[i]) \leq \text{Delta} * \text{card}(\text{Trans})$

easy to model

# How does it work ?

MODEL specifies task = constraints  
+ optimization criterion



Only state **WHAT** the problem is

Data = Input

## Solver I

- CP based
- Map to standard Solvers offered by Zinc
- Like Gecode and Comet
  - Gecode -- sound and complete
  - Comet -- local search ...
- CHALLENGE
  - how to encode this efficiently?



# Encoding in Zinc

```
int: Freq;
int: NrI; int: NrT;
array [1..NrT] of set of int: D;

array [1..NrI] of var bool: Items;
array [1..NrT] of var bool: Trans;

constraint % encode D: every Trans complement has no supported Items
forall(t in 1..NrT) (
  Trans[t] <-> sum(i in 1..NrI) ( Items[i]*(1 - (i in D[t])) ) <= 0
);

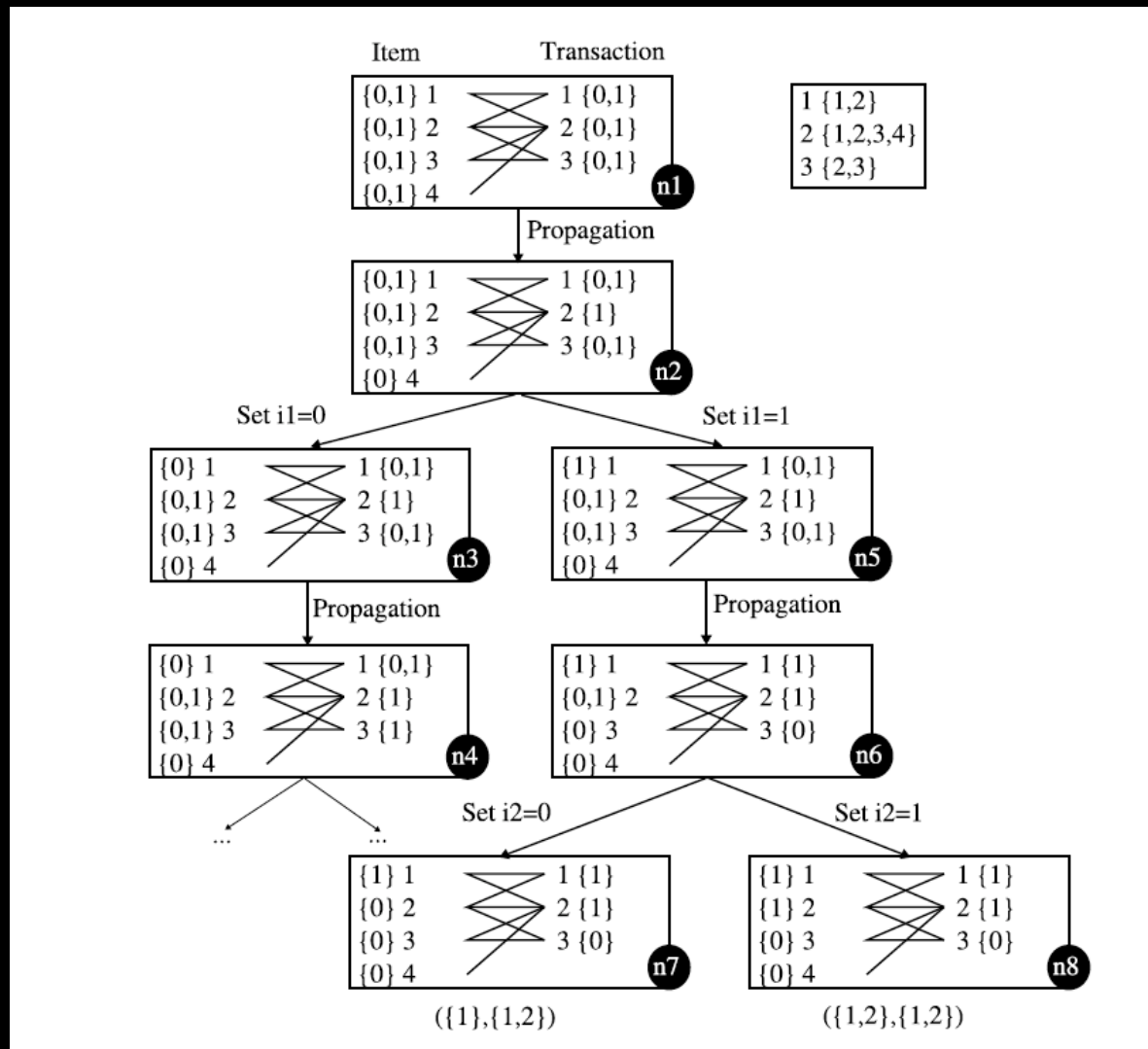
constraint % frequency: every Item is supported by sufficiently many Trans
forall(i in 1..NrI) (
  Items[i] -> sum(t in 1..NrT) ( Trans[t]*(i in D[t]) ) >= Freq
);

solve satisfy;
```

$$\forall t : T_t = 1 \Leftrightarrow \sum_i I_i (1 - D_{ti}) = 0$$

$$\sum_t T_t \geq \text{minsup} \quad \text{iff} \quad \forall_i^i : I_i = 1 \Rightarrow \sum_t T_t D_{ti} \geq \text{minsup}$$

# Resulting Search Strategy akin to Zaki's Eclat [KDD 97]



see  
Guns et al AIJ 11

## Solver 2

- Use a Data Mining System as solver
- Results with LCM [Uno et al.] within Zinc
- **CHALLENGE**
  - how to recognize that DM system applies ?
  - possibly add post-processing ...

B. Correlated Pattern Mining  
= Subgroup Discovery  
= Discriminative patterns

# Top-k Correlated Pattern Mining Subgroup Discovery

- $\mathcal{D}$  now consists of two datasets, say  $P$  and  $N$
- a correlation function  $\phi(p, \mathcal{D})$ , e.g.,  $\chi^2$
- $Th(\mathcal{L}, Q, \mathcal{D}) = \arg_{p \in \mathcal{L}} \max_k \phi(p, \mathcal{D})$

# Modeling perspective

→ **int: NrI; int: NrT; int: Freq;**  
**array[1..NrT] of set of int: D;**  
**set of int: pos; set of int: neg;**

**var set of 1..NrI: Items;**  
**var set of 1..NrT: Trans;**

**constraint Trans = cover(Items, D);**  
**constraint Items = cover\_inv(Trans, D);**

**solve maximize**

accuracy → **card(Trans intersect pos) – card(Trans intersect neg)**

Alternative opt. functions, for example:

**solve maximize chi2(Trans, pos, neg);**

with:

**function float: chi2(Trans, pos, neg)**

# Correlation function

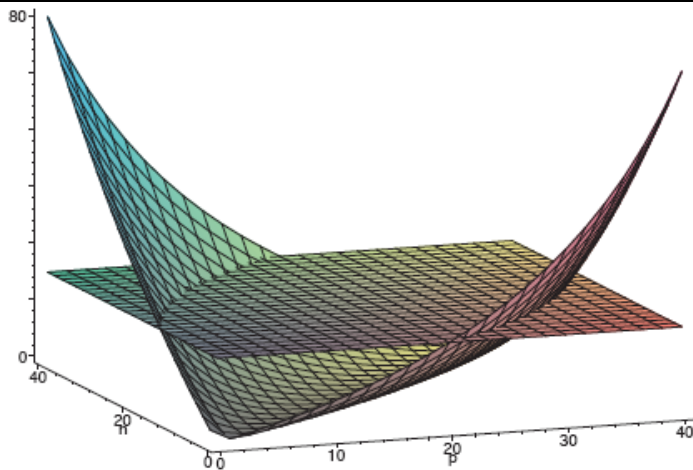
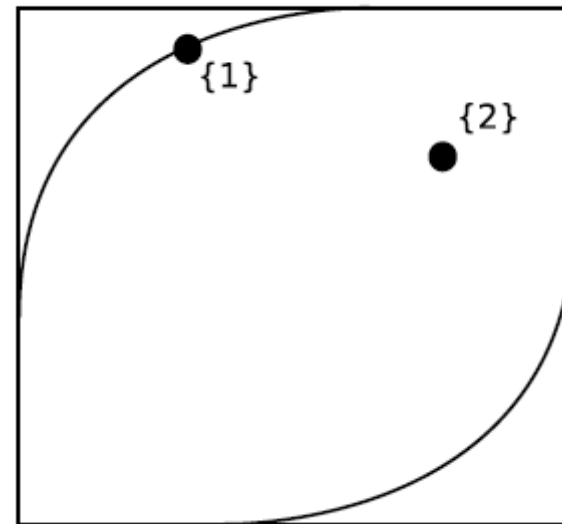


Figure 1: A plot of the  $\chi^2$  scoring function, and a threshold on  $\chi^2$ .



Projection on PN-space  
Nijssen KDID

# Monotonicity

$$\text{freq}(S) \geq \text{freq}(S \cup T) \geq \text{freq}(S \cup \text{Dom}(S))$$

Traditional pruning/propagation employs **upper bound**:

remove  $d$  from  $\text{Dom}(S)$  when  $\text{freq}(S) \geq t$  and  $\text{freq}(S \cup \{d\}) < t$

Other propagation – unavoidable item sets also possible – **lower bound**

$$\text{freq}(S) \geq \text{freq}(S \cup T) \geq \text{freq}(S \cup \text{Dom}(S)) = a > 0$$

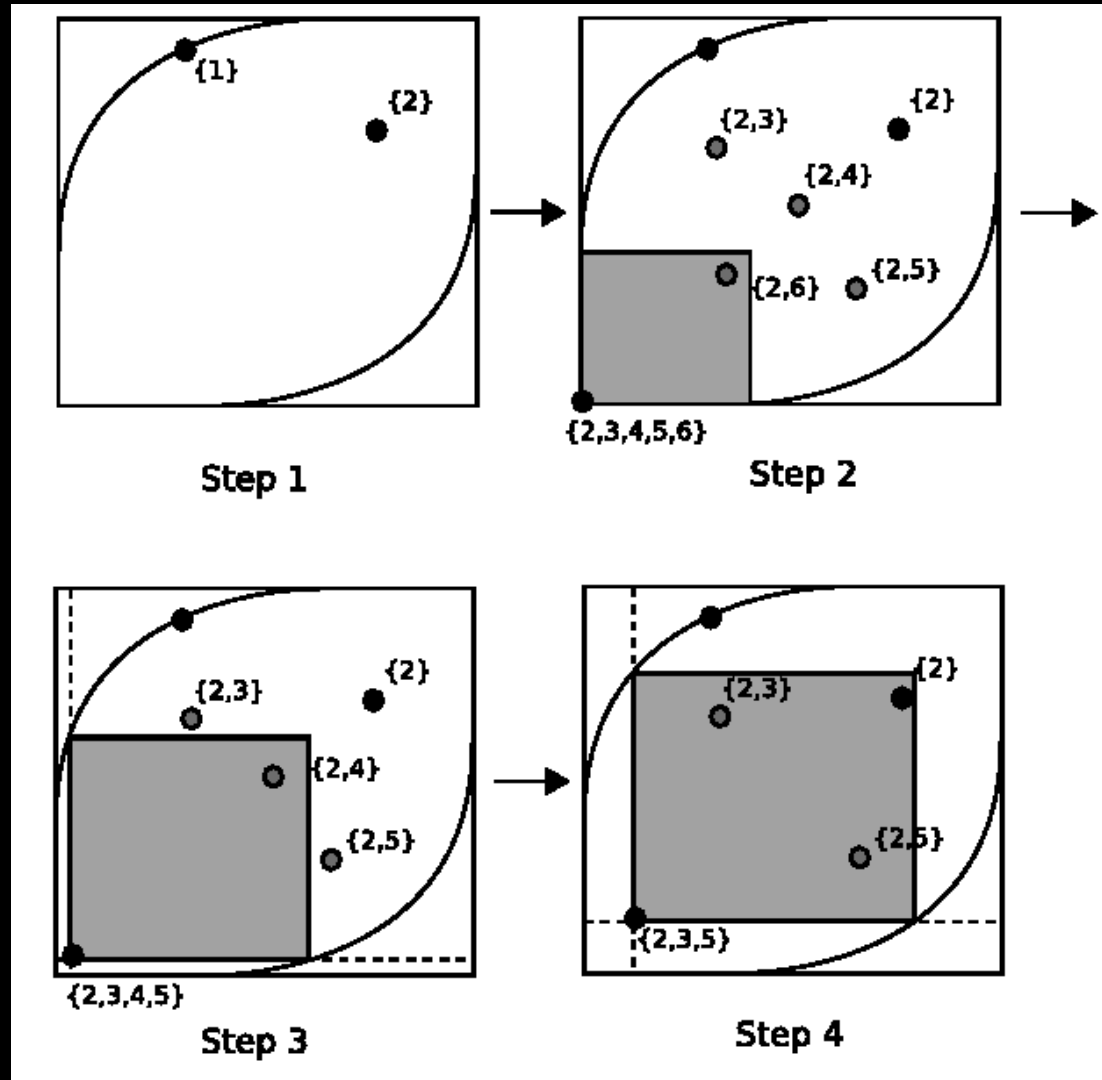
then  $a$  is a lower bound on  $\text{freq}(S)$ , that is  $\text{freq}(S) \geq a$

**Solving using CP can be extremely effective**

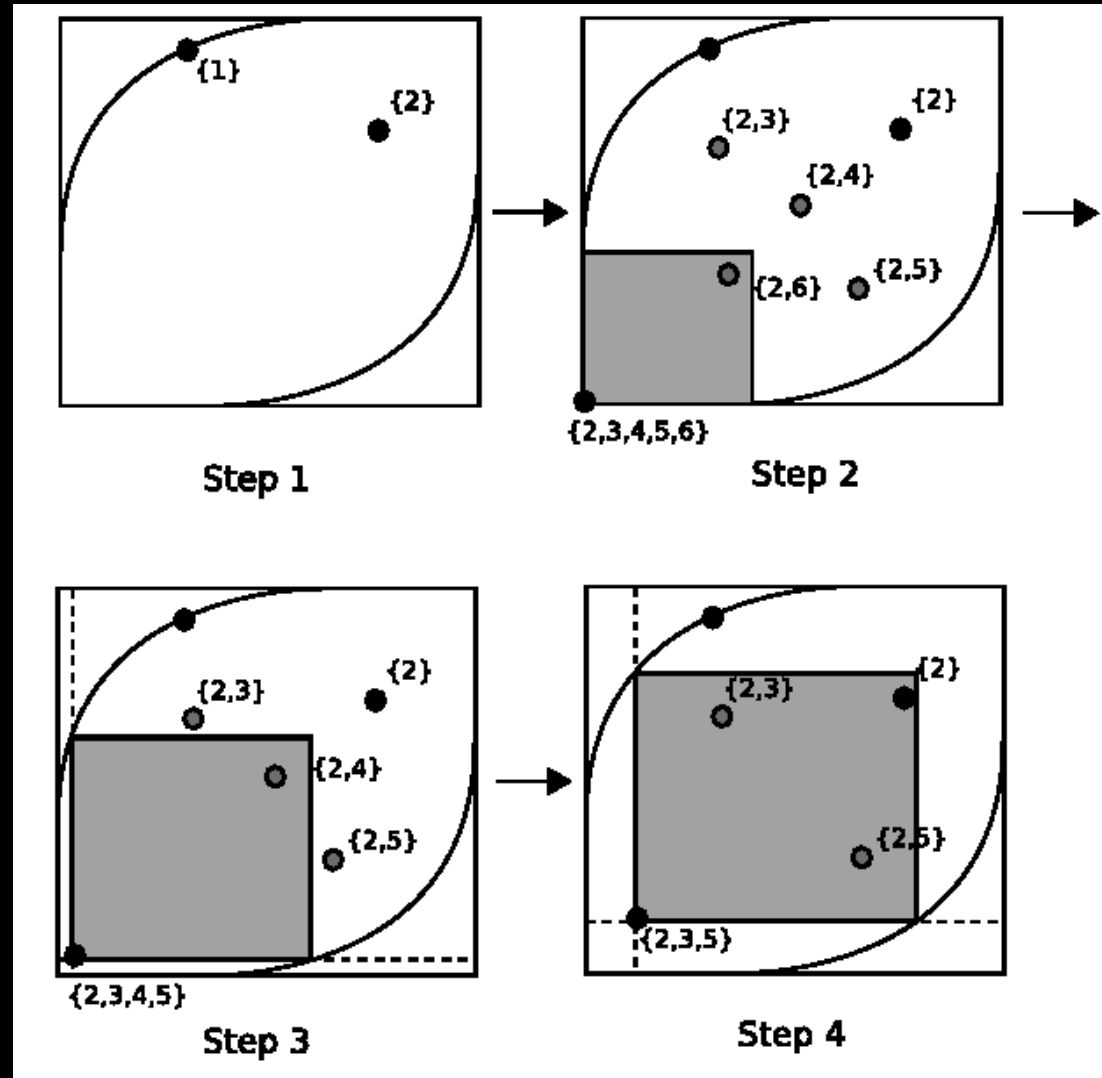


# Illustration

$$\text{Dom}(\{2\}) = \{2,3,4,5,6\}$$

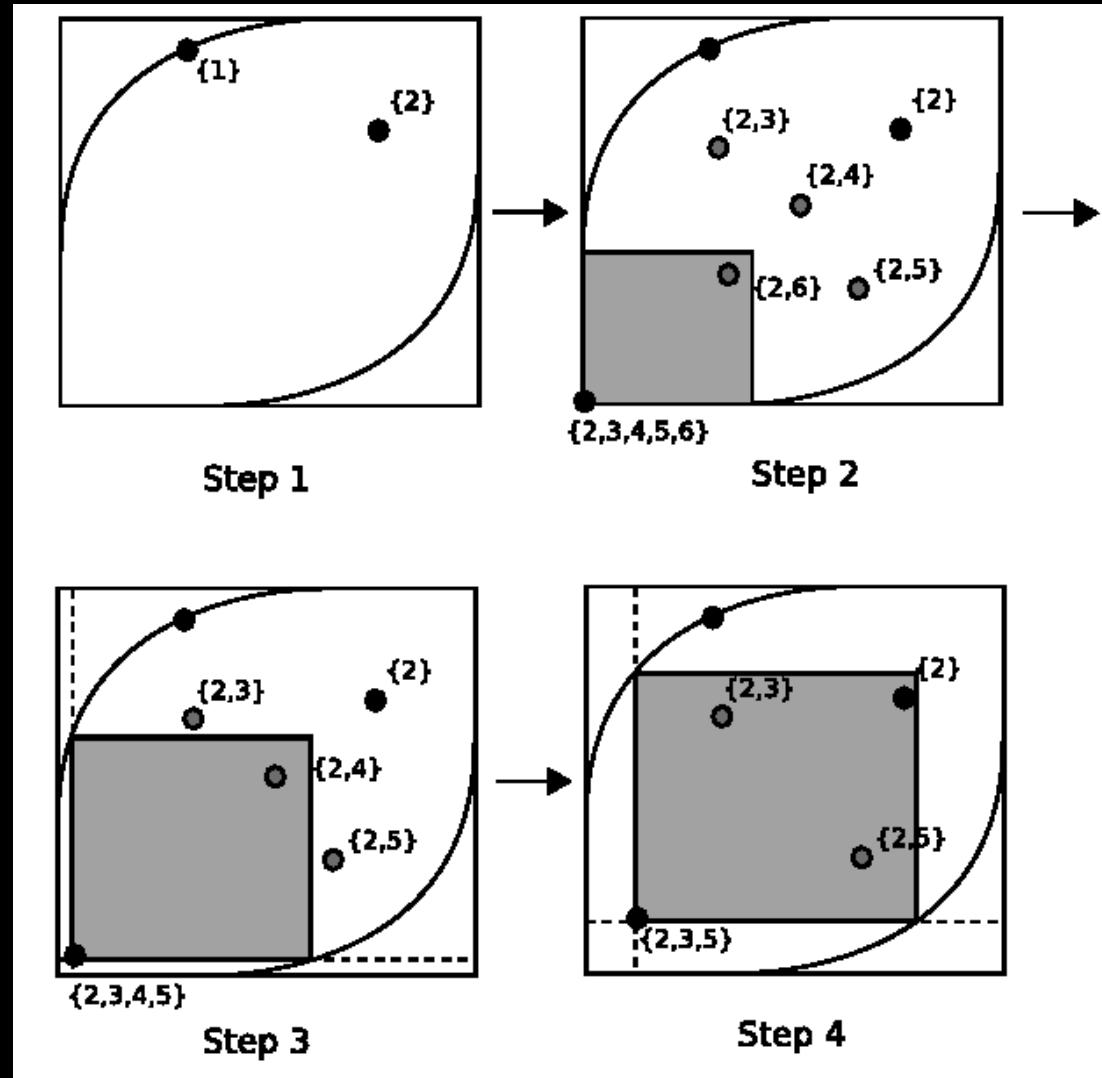


# Illustration



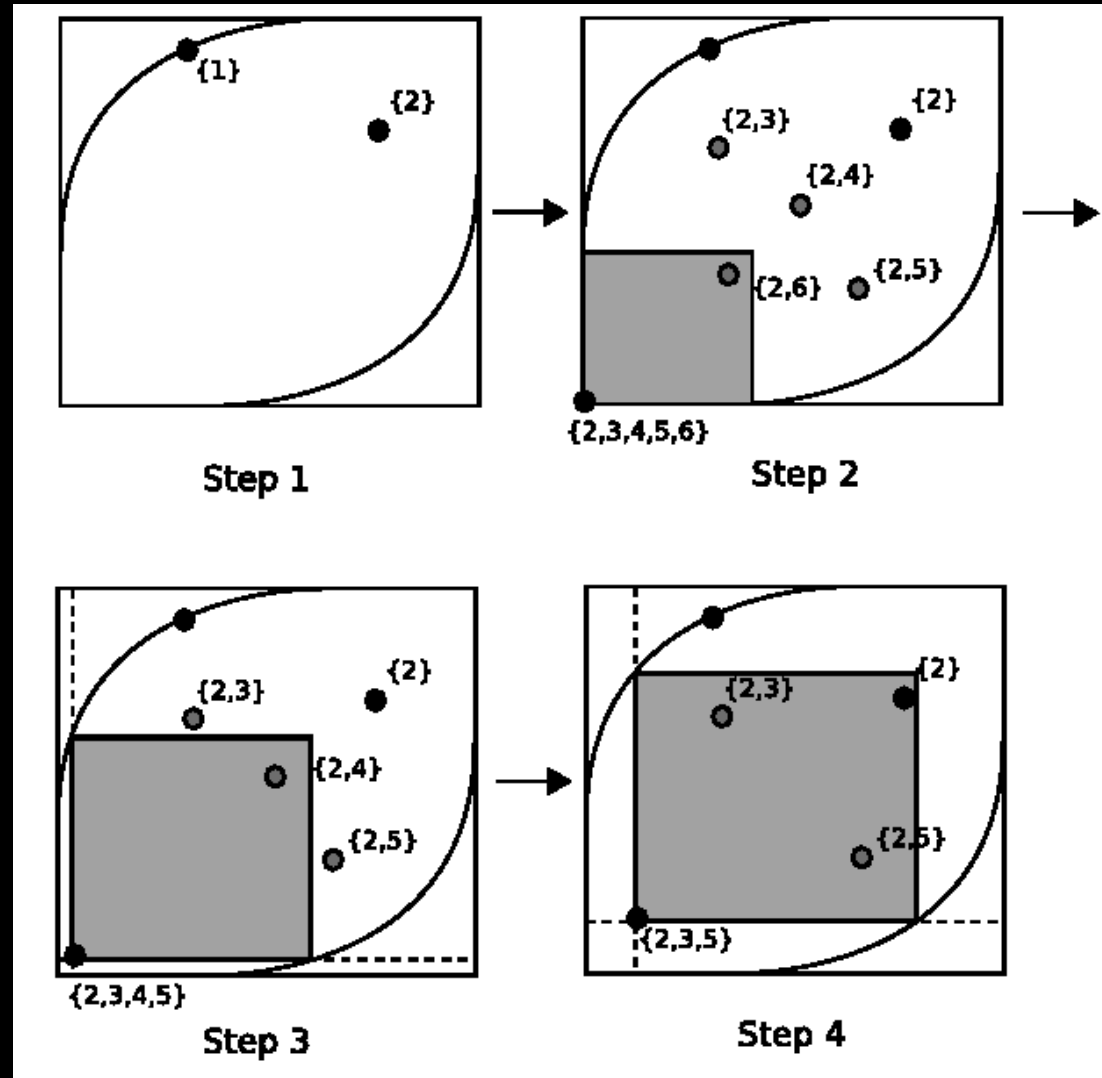
$$\text{Dom}(\{2\}) = \{2, 3, 4, 5\}$$

# Illustration



$$\text{Dom}(\{2\}) = \{2,3,5\}$$

# Illustration



$$\text{Dom}(\{2\}) = \{ \}$$

# 4-support bound

Nijssen et  
al. KDD 09  
AIJ 11

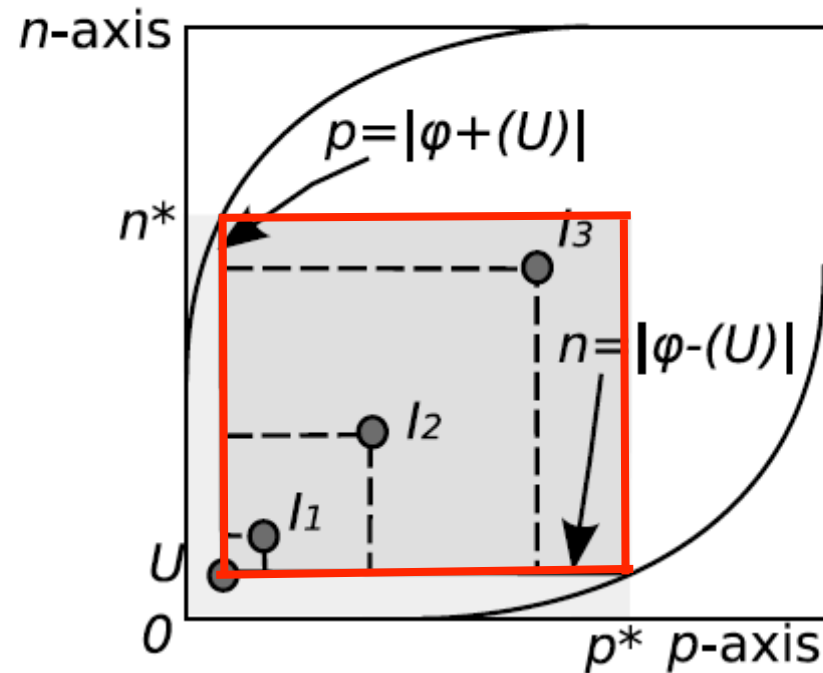


Figure 4: The 4-support bound in PN-space.

# 2-support bound

Morishita &  
Sese  
SIGMOD98

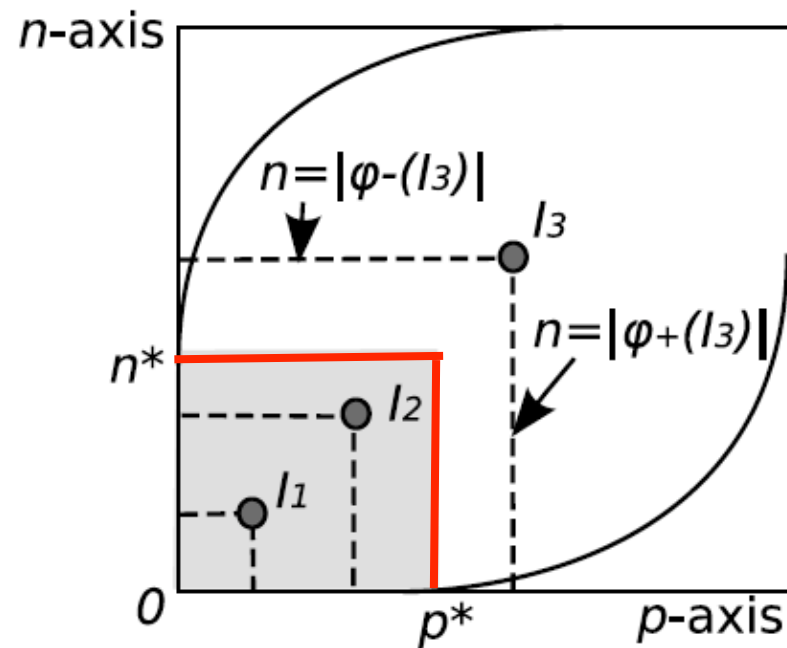
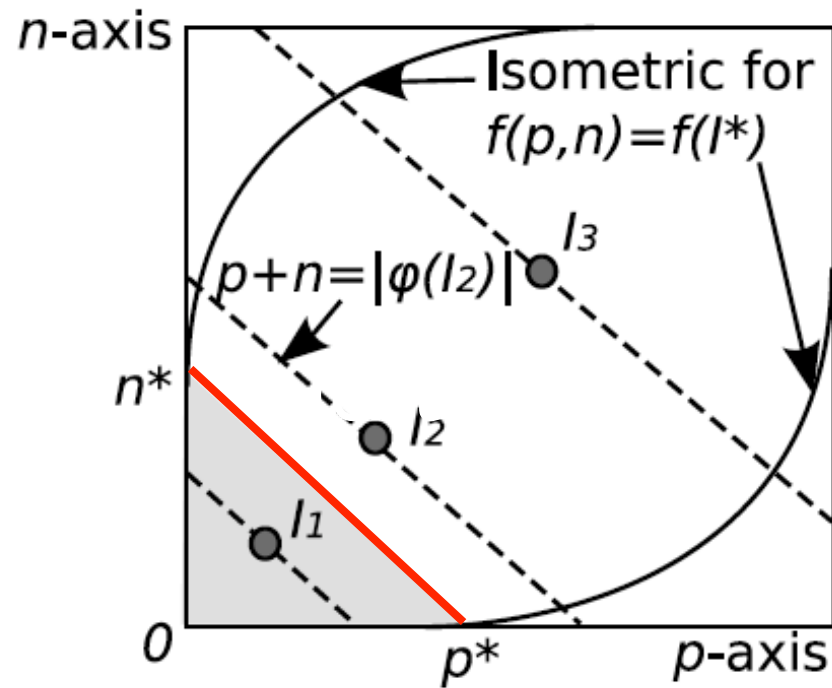


Figure 3: The 2-support bound in  $PN$ -space.

# 1-support bound



Han et al.  
ICDM 08

Figure 2: The 1-support bound in PN-space.

# Experiments

Name	Density	4-supp.	2-supp.	1-supp.
anneal	0.45	0.22	24.09	72.71
australian-credit	0.41	0.30	0.63	17.52
breast-wisconsin	0.5	0.28	13.66	228.08
diabetes	0.5	2.45	128.04	>
german-credit	0.34	2.39	66.79	>
heart-cleveland	0.47	0.19	2.15	29.58
hypothyroid	0.49	0.71	10.91	>
ionosphere	0.5	1.44	>	>
kr-vs-kp	0.49	0.92	46.20	713.35
letter	0.5	52.66	>	>
mushroom	0.18	14.11	13.48	27.31
pendigits	0.5	3.68	>	>
primary-tumor	0.48	0.03	0.13	0.85
segment	0.5	1.45	>	>
soybean	0.32	0.05	0.07	0.38
splice-1	0.21	30.41	31.11	35.02
vehicle	0.5	0.85	>	>
yeast	0.49	5.67	781.63	>

900s  
timeout

Solving using CP can be extremely effective



# C. Pattern Set Mining

# Pattern Sets

$$Th(\mathcal{L}, Q, \mathcal{D}) = \{P \subseteq \mathcal{L} \mid Q(P, \mathcal{D}) = true\}$$

One is not interested in all solutions to a pattern mining task, typically post-processing needed

So, why not apply constraint based mining to pattern sets directly? [Zimmermann 09]  
[Guns et al, IEEE TKDE 11]

# Pattern Sets

Consider a set of itemsets

$$\{\{a, b, c\}, \{b, d, e\}, \{c, e, f\}\}$$

Can be interpreted as DNF expression

$$(a \wedge b \wedge c) \vee (b \wedge d \wedge e) \vee (c \wedge e \wedge f)$$

Useful for concept-learning and clustering

from local to global pattern mining

# Pattern Sets

$$Th(\mathcal{L}, Q, \mathcal{D}) = \{P \subseteq \mathcal{L} \mid Q(P, \mathcal{D}) = true\}$$

What are meaningful constraints ?

- local constraints on  $I \in P$  such as  $freq(I, \mathcal{D}) \geq minsup$
- constraints on all pairs of patterns  $I_1, I_2 \in P$ , e.g.  
 $|covers(I_1, \mathcal{D}) \cap covers(I_2, \mathcal{D})| \leq t$
- global constraints  $freq(P, \mathcal{D}) \geq t'$
- correlation, top-k, ...

# k-*Pattern Set* Mining ( $|P|=k$ )

```
int: NrI; int: NrT;      int K;  
array[1..NrT] of set of int: D;  
set of int: pos; set of int: neg;  
  
% pattern set  
array[1..K] of var set of 1..NrI: Items;  
constraint lexleq(Items); % remove symmetries  
  
% every pattern is closed 'on the positives'  
constraint let { Dp = [D[t] | t in pos] } in  
    forall (d in 1..K) (  
        Items[d] = cover_inv(cover(Items[d], Dp), Dp));  
  
% accuracy of pattern set  
solve maximize  
    let { Trans = union(d in 1..K) (cover(Items[d], D)) } in  
    card(Trans intersect pos) - card(Trans intersect neg);
```

# Generality

Can model instantiations/versions of:

- Concept learning (k-term DNF learning)
- Conceptual clustering
- k-Tiling
- Redescription mining
- ...

# Pattern Mining

## A. frequent pattern

- which patterns are frequent ?

$$Th(\mathcal{L}, Q, \mathcal{D}) = \{P \in \mathcal{L} \mid Q(P, \mathcal{D}) \geq \theta\}$$

## B. Correlated pattern

- which patterns are correlated ?

We have been using off-the-shelf CP SOLVERS for these tasks, cf. Guns, Nijssen, De Raedt [AAAI 10, AIJ 11]

One solver for all of these

Easy to combine different constraints

Now looking at modeling level

KDD 08

KDD 09

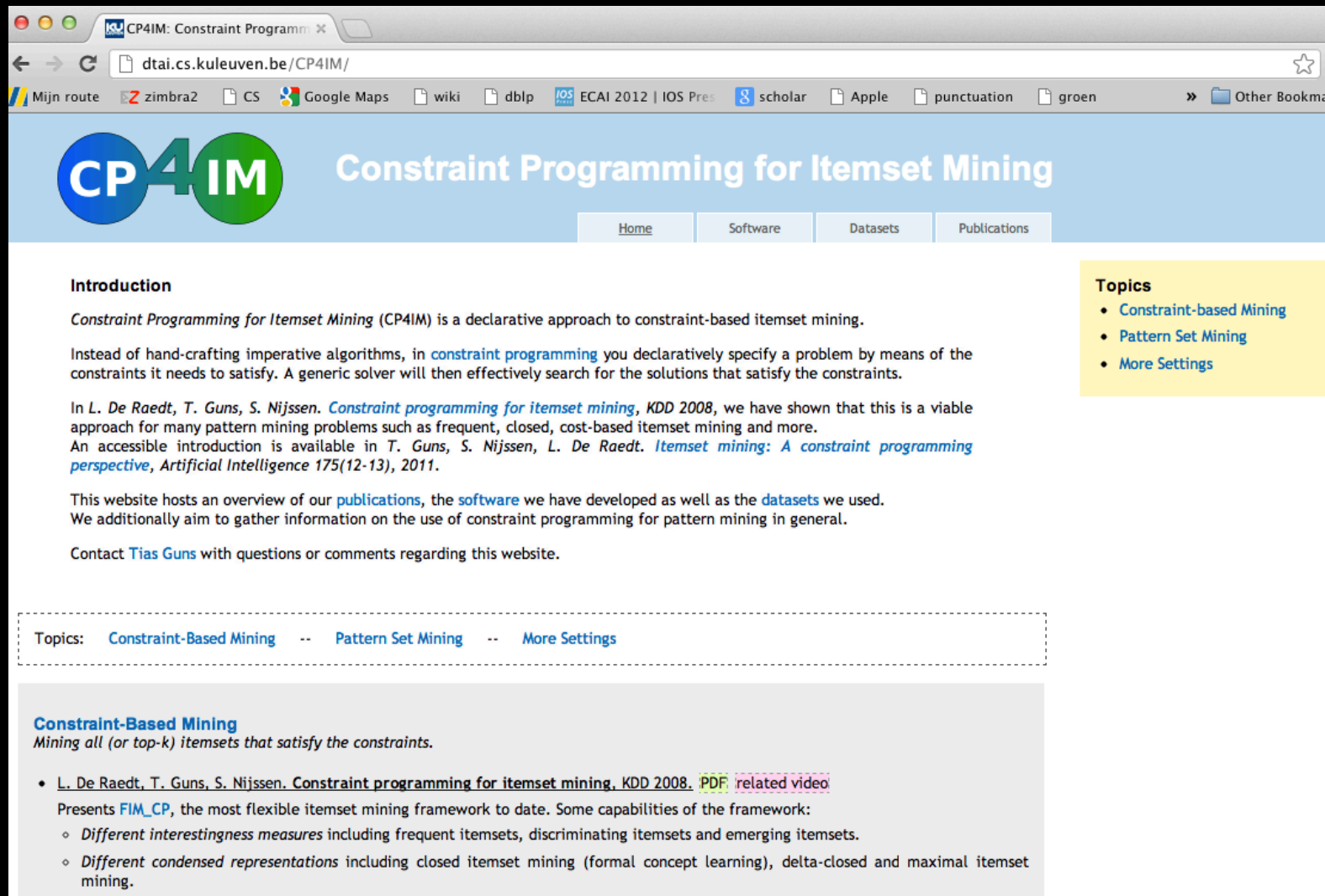
## C. pattern

- which patterns are concept-descriptions for the actives ?  
for the

$$Th(\mathcal{L}, Q, \mathcal{D}) = \{P \subseteq \mathcal{L} \mid Q(P, \mathcal{D}) = true\}$$

IEEETKDE 11

# http://dtai.cs.kuleuven.be/CP4IM



The image shows a screenshot of a web browser displaying the homepage of the CP4IM project. The browser's address bar shows the URL [dtai.cs.kuleuven.be/CP4IM/](http://dtai.cs.kuleuven.be/CP4IM/). The website has a light blue header with the CP4IM logo (CP in a blue circle, 4 in a green circle, IM in a green circle) and the title "Constraint Programming for Itemset Mining". Below the header is a navigation menu with links for "Home", "Software", "Datasets", and "Publications". The main content area is titled "Introduction" and contains several paragraphs of text. On the right side, there is a yellow box titled "Topics" with three bullet points: "Constraint-based Mining", "Pattern Set Mining", and "More Settings". At the bottom of the page, there is a dashed box containing the text "Topics: Constraint-Based Mining -- Pattern Set Mining -- More Settings". Below this, there is a section titled "Constraint-Based Mining" with a sub-heading "Mining all (or top-k) itemsets that satisfy the constraints." and a list of bullet points.

**CP4IM** Constraint Programming for Itemset Mining

[Home](#) [Software](#) [Datasets](#) [Publications](#)

### Introduction

*Constraint Programming for Itemset Mining (CP4IM)* is a declarative approach to constraint-based itemset mining.

Instead of hand-crafting imperative algorithms, in [constraint programming](#) you declaratively specify a problem by means of the constraints it needs to satisfy. A generic solver will then effectively search for the solutions that satisfy the constraints.

In [L. De Raedt, T. Guns, S. Nijssen. \*Constraint programming for itemset mining\*, KDD 2008](#), we have shown that this is a viable approach for many pattern mining problems such as frequent, closed, cost-based itemset mining and more. An accessible introduction is available in [T. Guns, S. Nijssen, L. De Raedt. \*Itemset mining: A constraint programming perspective\*, Artificial Intelligence 175\(12-13\), 2011](#).

This website hosts an overview of our [publications](#), the [software](#) we have developed as well as the [datasets](#) we used. We additionally aim to gather information on the use of constraint programming for pattern mining in general.

Contact [Tias Guns](#) with questions or comments regarding this website.

Topics: [Constraint-Based Mining](#) -- [Pattern Set Mining](#) -- [More Settings](#)

### Constraint-Based Mining

Mining all (or top-k) itemsets that satisfy the constraints.

- [L. De Raedt, T. Guns, S. Nijssen. \*Constraint programming for itemset mining\*, KDD 2008. \[PDF\]\(#\) \[related video\]\(#\)](#)  
Presents [FIM\\_CP](#), the most flexible itemset mining framework to date. Some capabilities of the framework:
  - Different interestingness measures* including frequent itemsets, discriminating itemsets and emerging itemsets.
  - Different condensed representations* including closed itemset mining (formal concept learning), delta-closed and maximal itemset mining.



Perspective

# All this is fine but...

what about

- efficiency and scalability ?
- other types of data and patterns (sequences, trees, graphs ...) ? **relational**
- other DM/ML tasks ? **probabilistic, statistical learning, kernels / distances ...**

# Efficiency / Scalability

- Trade-off efficiency / generality
- Current experiments (with ONE solver)
  - Often a constant factor slower
  - Some cases much faster (correlated)
  - Avoid with specialized solvers [Nijssen and Guns, ECMLPKDD 10]
- Feature of Declarative Modeling
  - many solvers available (complete, approximate, ... )
  - one can even work with portfolio's (Satzilla)
- Challenge is to build **efficient solvers and translations**

**The new role of DM/ML scientists if we succeed ?**

# Task / Representation

Rich representations ~ relational, graphs ?

Task level ~ unsupervised, regression, clustering, probabilistic... ?

Let us have a look at Statistical Relational Learning

Markov Logic [Domingos et al.]

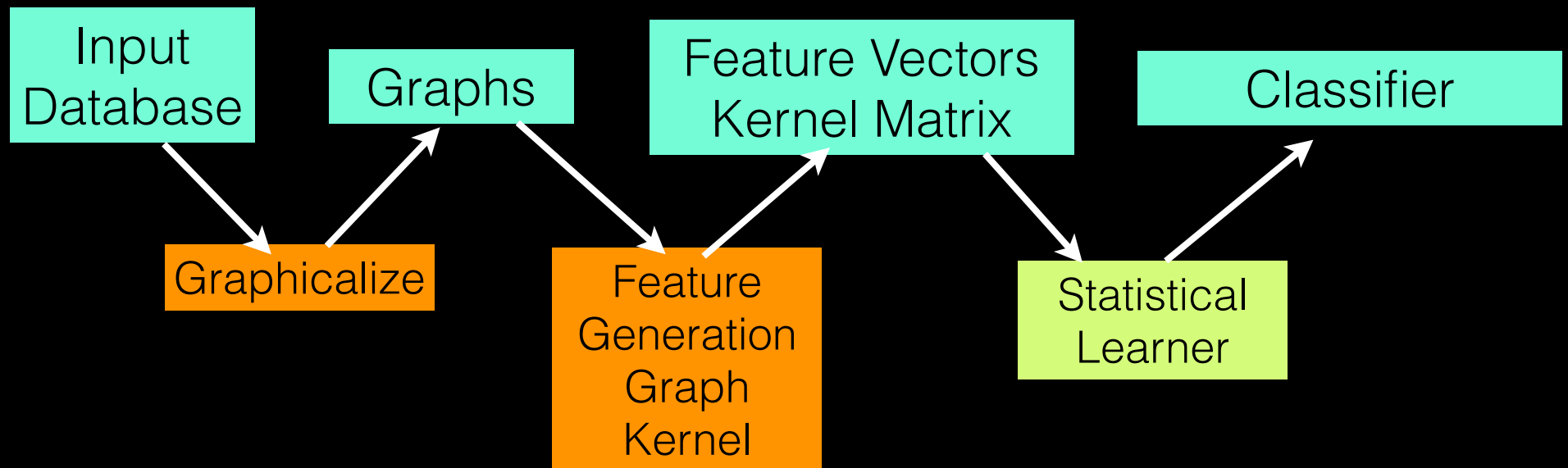
ProbLog [De Raedt et al.]

...

kLog [Frasconi et al.] kernel based

probabilistic

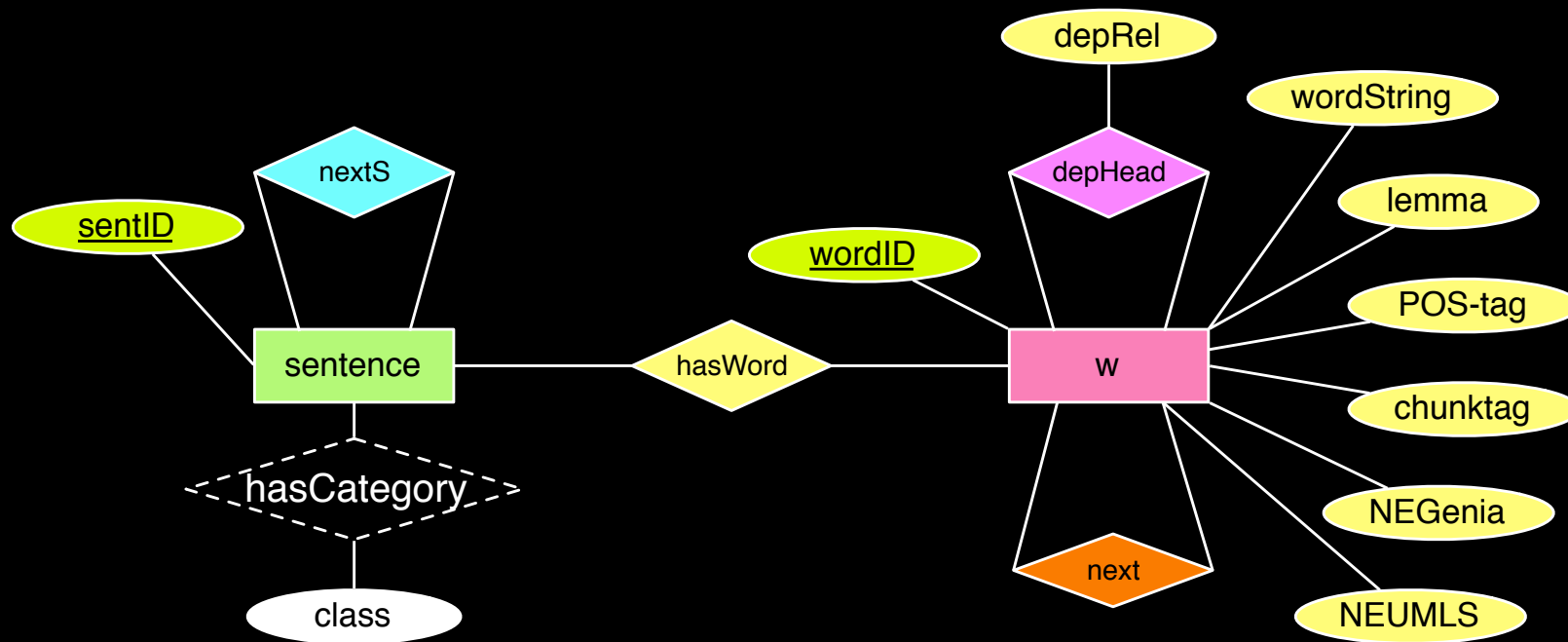
# kLOG [Frasconi, Costa, DR, De Grave 12]



# A biomedical NLP task [Verbeke et al. EMLNP 12]

Surgical excision of CNV may allow stabilisation or improvement of vision .

# E/R-MODEL



[Verbeke et al. EMNLP 12]

# Relational ....

```
sentence(s4,4).
hasCategory(s4,'background').
w(w4_1,'Surgical','Surgical',b-np,jj,'O','O').
hasWord(s4,w4_1).
dh(w4_1,w4_2,nmod).
nextW(w4_2,w4_1).
w(w4_2,'excision','excision',i-np,nn,'O','O').
hasWord(s4,w4_2).
dh(w4_2,w4_5,sub).
nextW(w4_3,w4_2).
w(w4_3,'of','of',b-pp,in,'O','O').
hasWord(s4,w4_3).
dh(w4_3,w4_2,nmod).
nextW(w4_4,w4_3).
w(w4_4,'CNV','CNV',b-np,nn,'B-protein','O').
hasWord(s4,w4_4).
dh(w4_4,w4_3,pmod).
nextW(w4_5,w4_4).
w(w4_5,'may','may',b-vp,md,'O','O').
hasWord(s4,w4_5).
dh(w4_5,w4_0,root).
nextW(w4_6,w4_5).
```

```
lemmaRoot(S,L):-
    hasWord(S,l), w(l,_L,_,_,_), dh(l_,root).
```

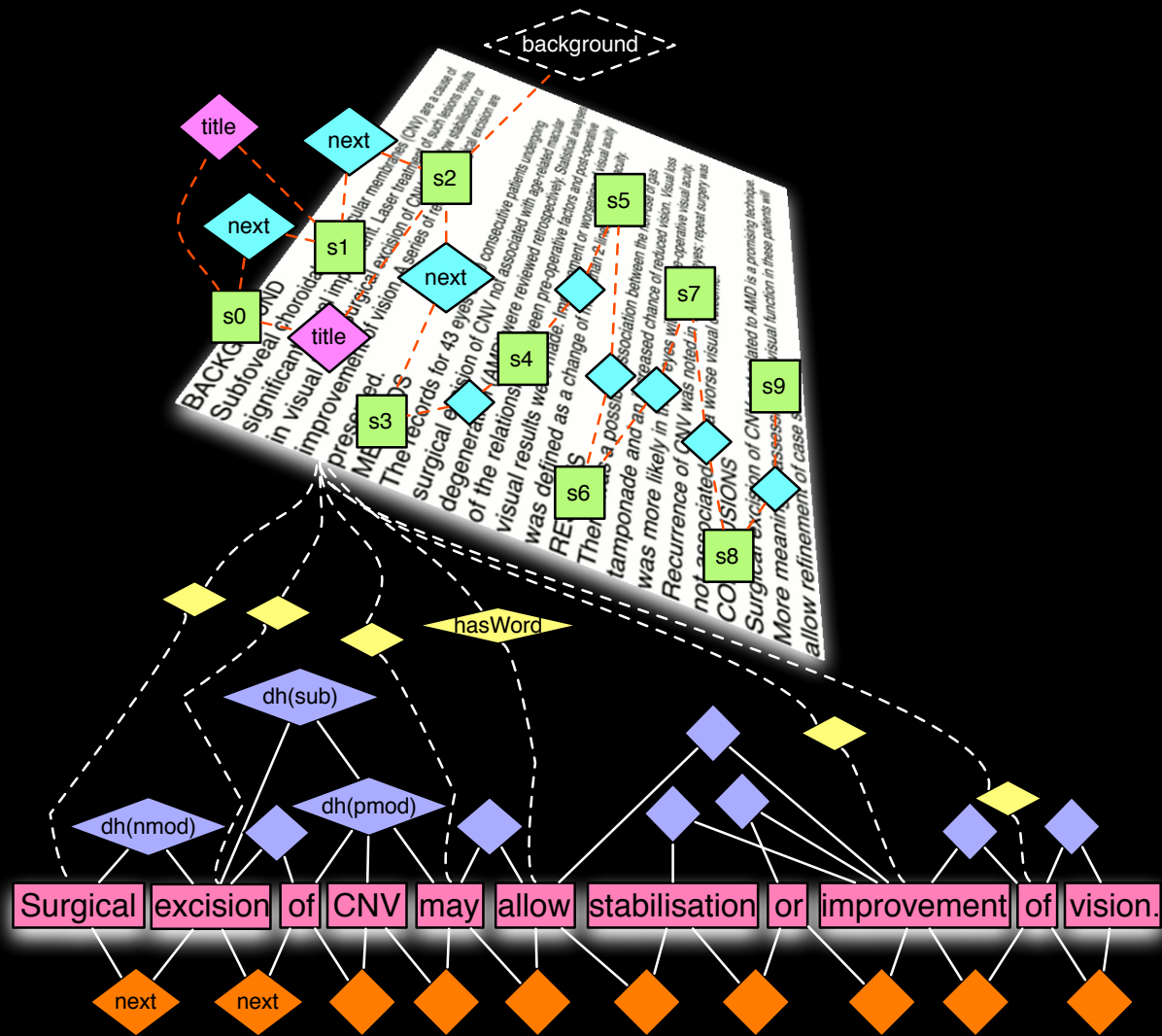
```
isHeaderSentence(S):-
    hasHeaderWord(S,_).
```

```
hasSectionHeader(S,X):-
    nextS(SI,S),
    hasHeaderWord(SI,X),!.
```

```
hasSectionHeader(S,X):-
    nextS(SI,S),
    \+isHeaderSentence(S),
    once(hasSectionHeader(SI,X)),!.
```

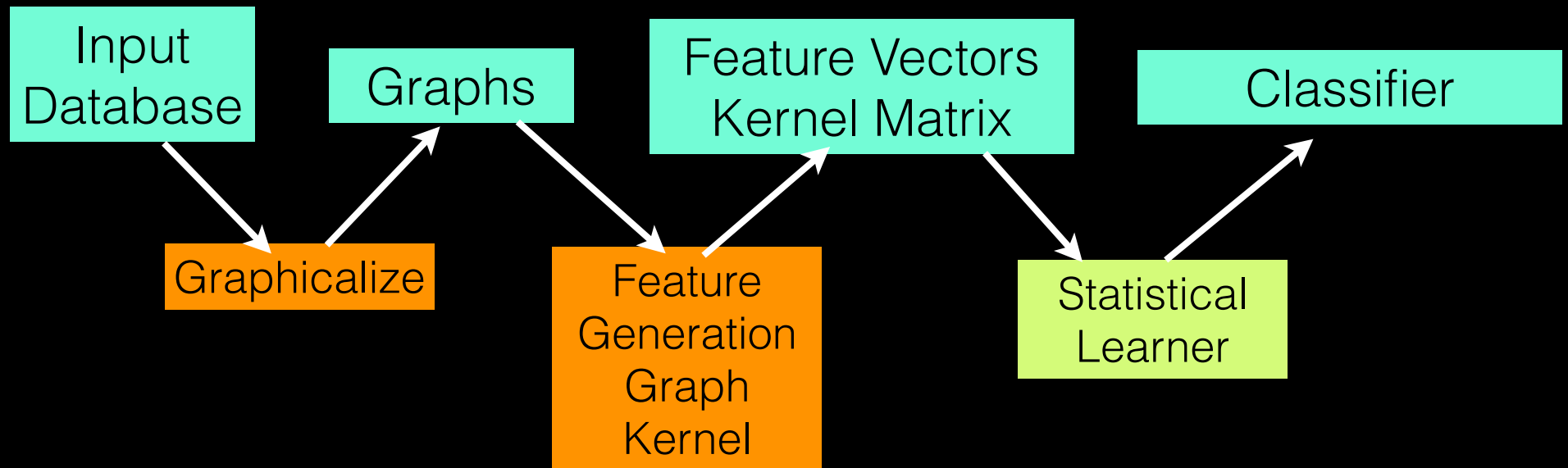
...  
relational database ... Prolog

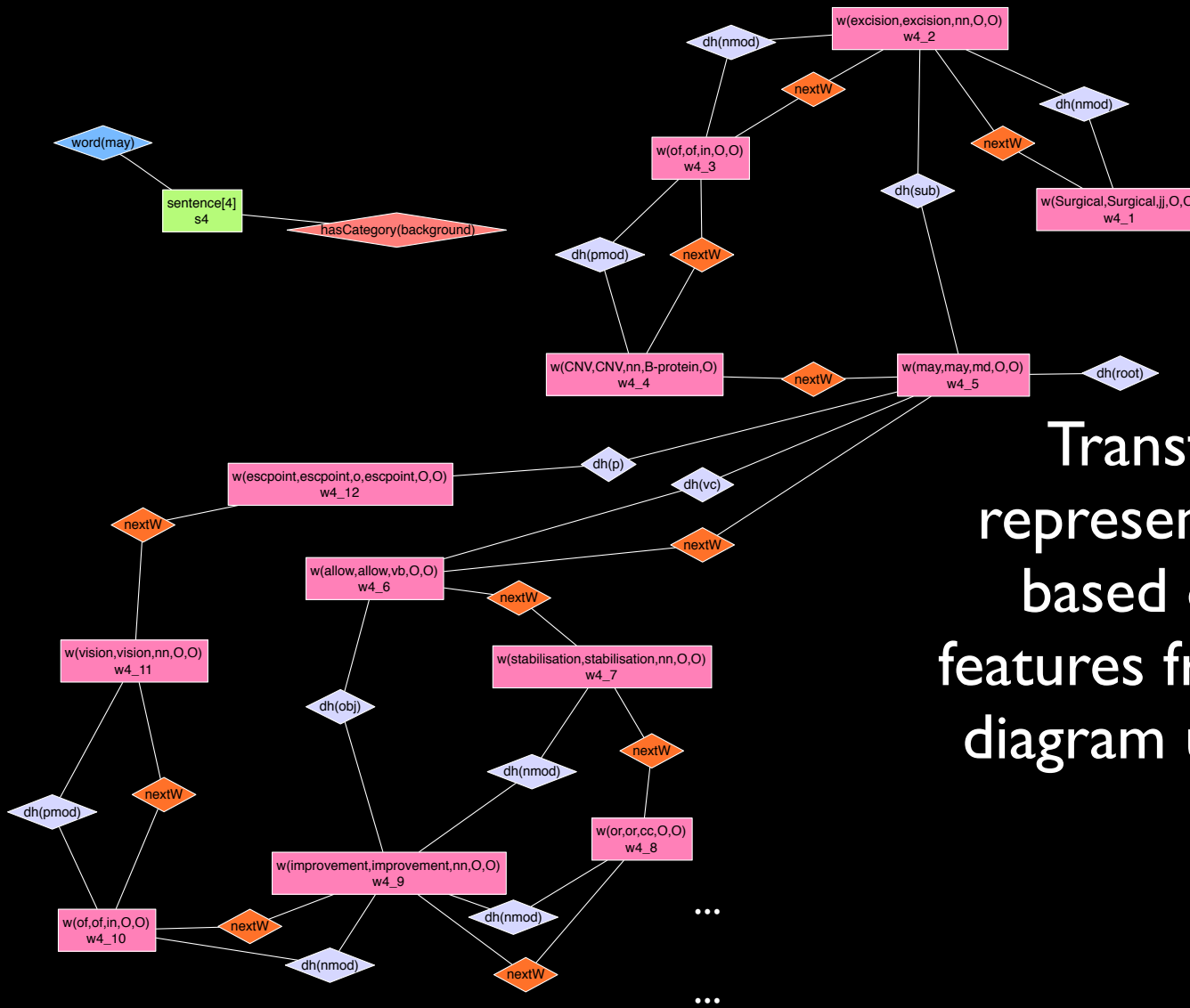




# Graphicalization

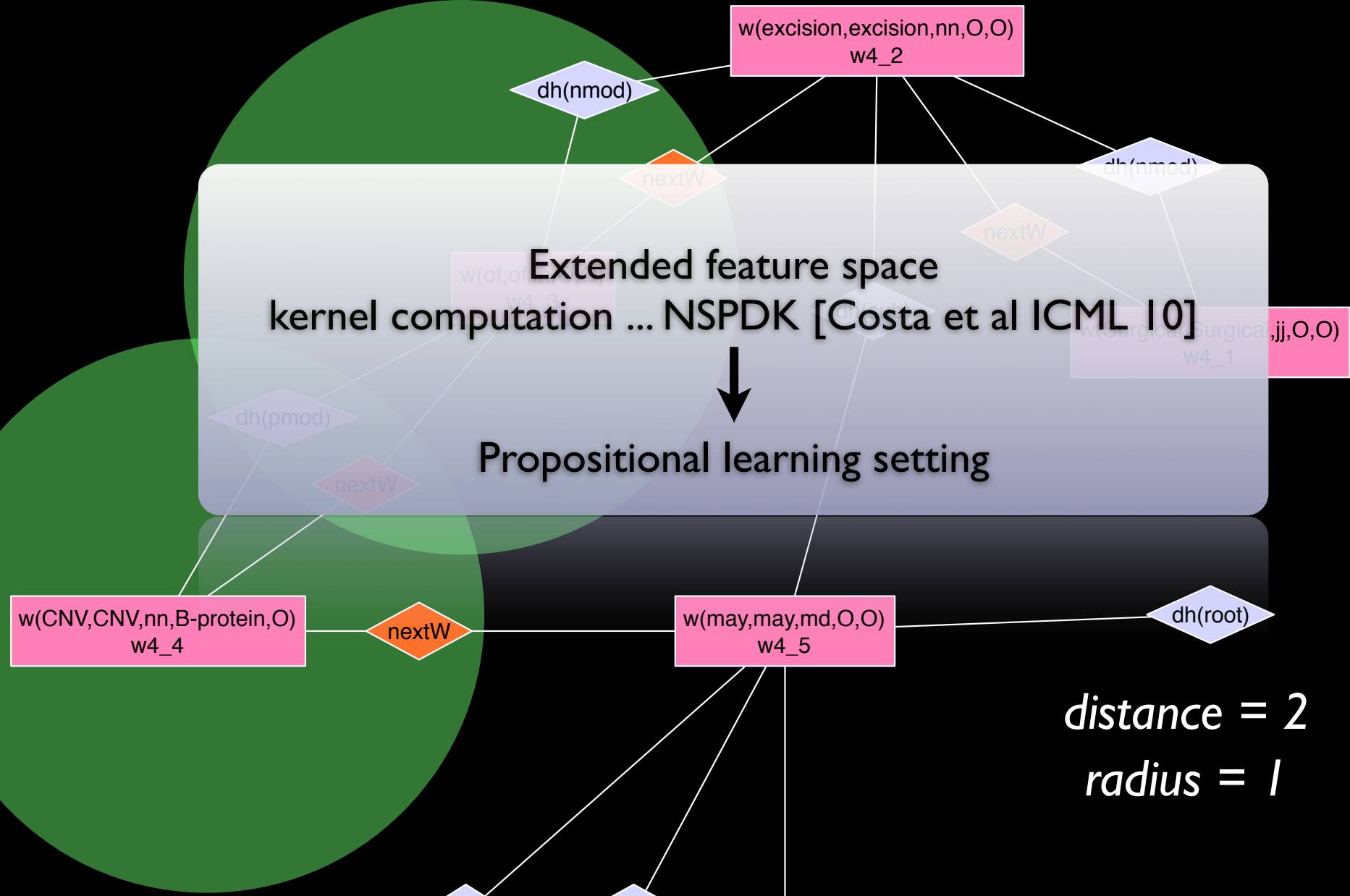
# KLOG



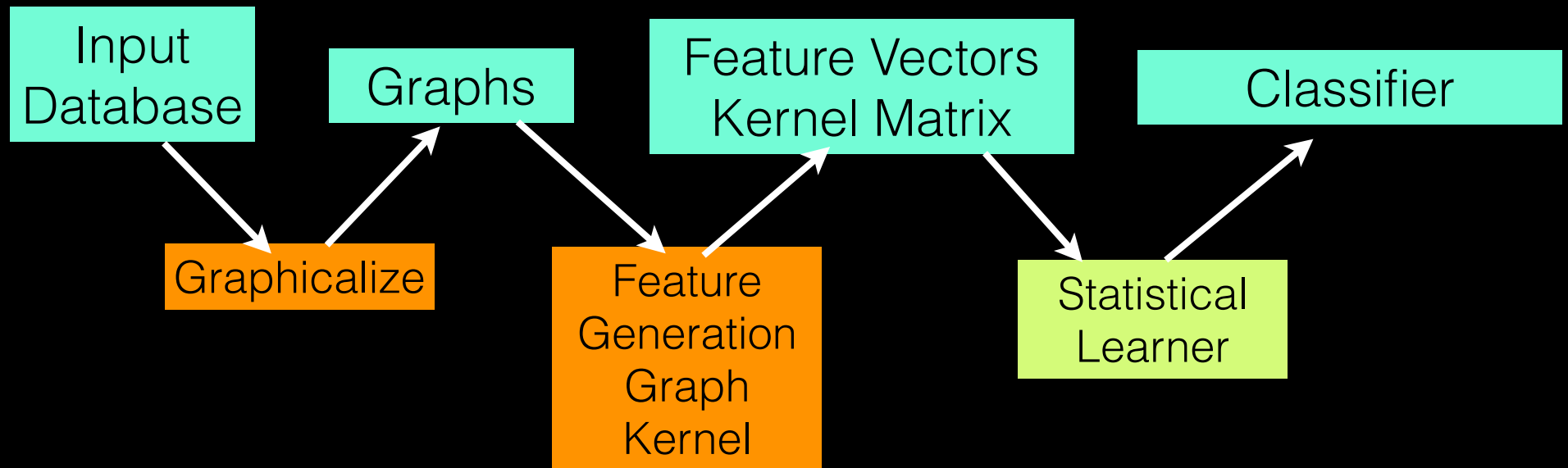


Transforms relational representations into graph based ones and derives features from a grounded E/R diagram using graph kernels

...



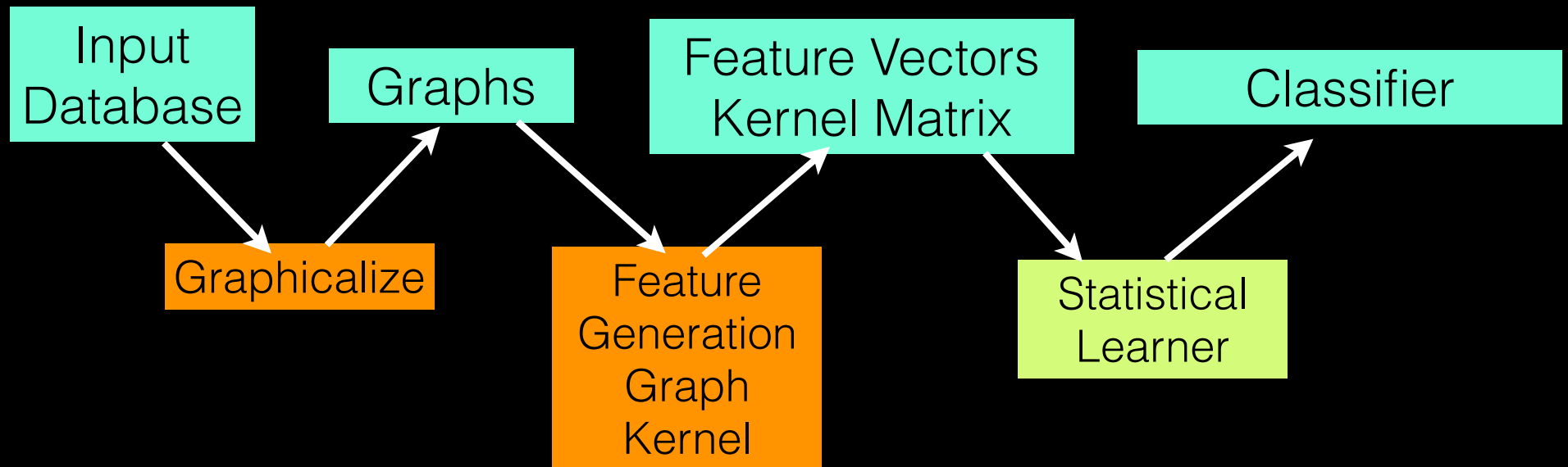
# KLOG



# kLOG

Task

Task MODEL specifies task =  
constraints + optimization criterion

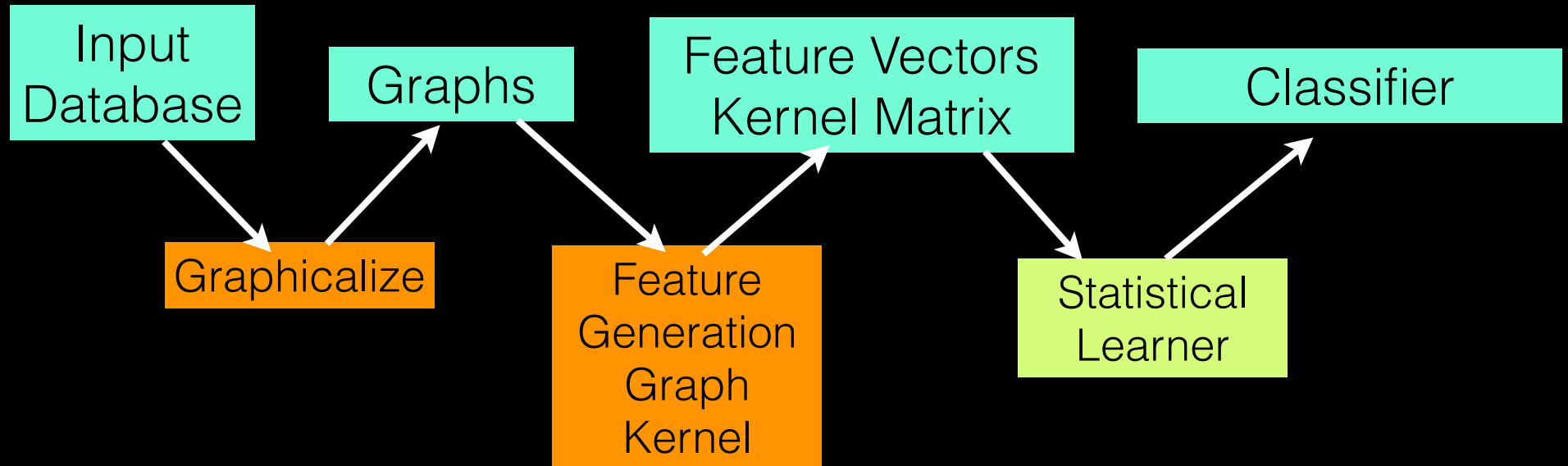


# kLOG

## CHALLENGE

Define the KERNEL declaratively  
Define the LOSS function ... and SOLVE

Task



As for many other ML/DM systems ?

What if we succeed ?



# Our work today ...

We typically ...

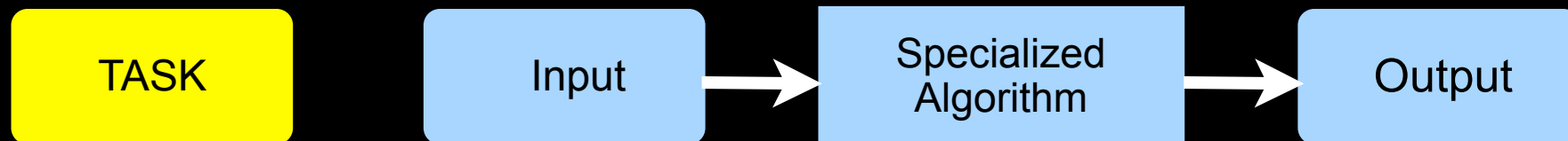
1. Formalize learning / mining task

2. Design algorithm / technique to use

hard

3. Implement the algorithm

4. Use and distribute the software



# Our work tomorrow ...

The **user/application** perspective...

1. Formalize learning / mining task

2. Model the problem

**easy**

3. Select the right solvers

4. Use and distribute the software

More opportunities for re-use ...

A de facto standard language for DM / ML as Zinc ?

# Our work tomorrow ...

The **scientist's** perspective...

Designing modeling languages

Studying task properties

**more fun**

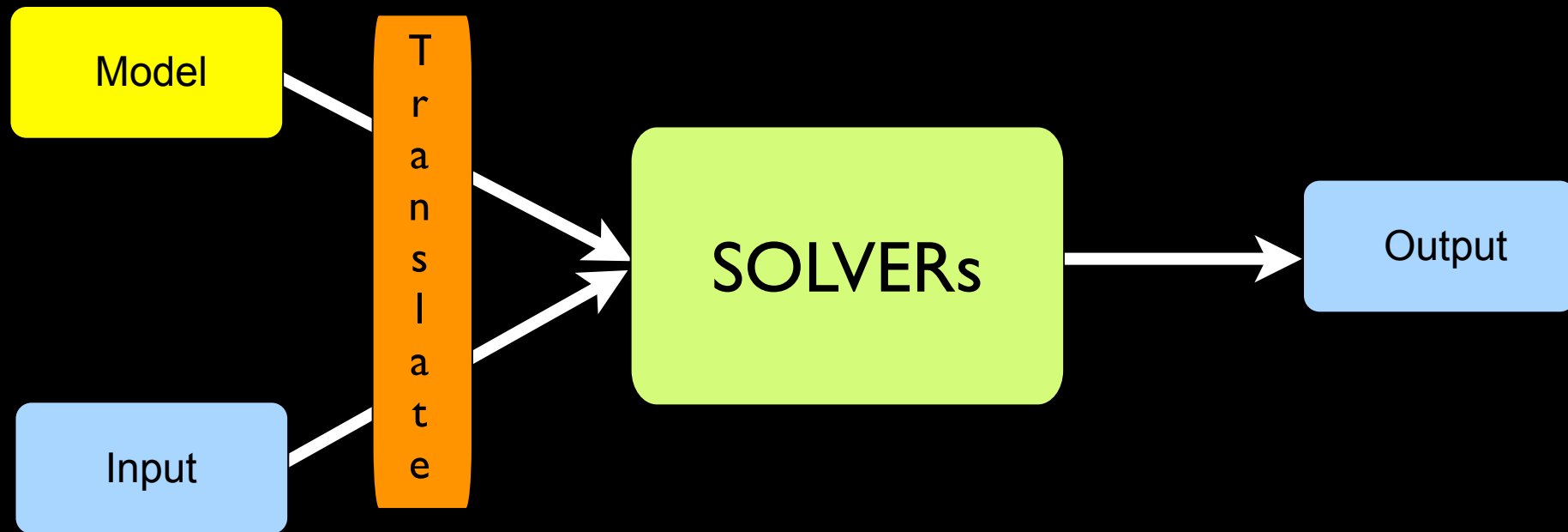
Studying translations

Producing and adapting solvers

Larger impact of results in larger framework ?

# Conclusions

Declarative modeling languages for ML / DM has high potential



Embedding in programming languages may provide an answer to Mitchell's question

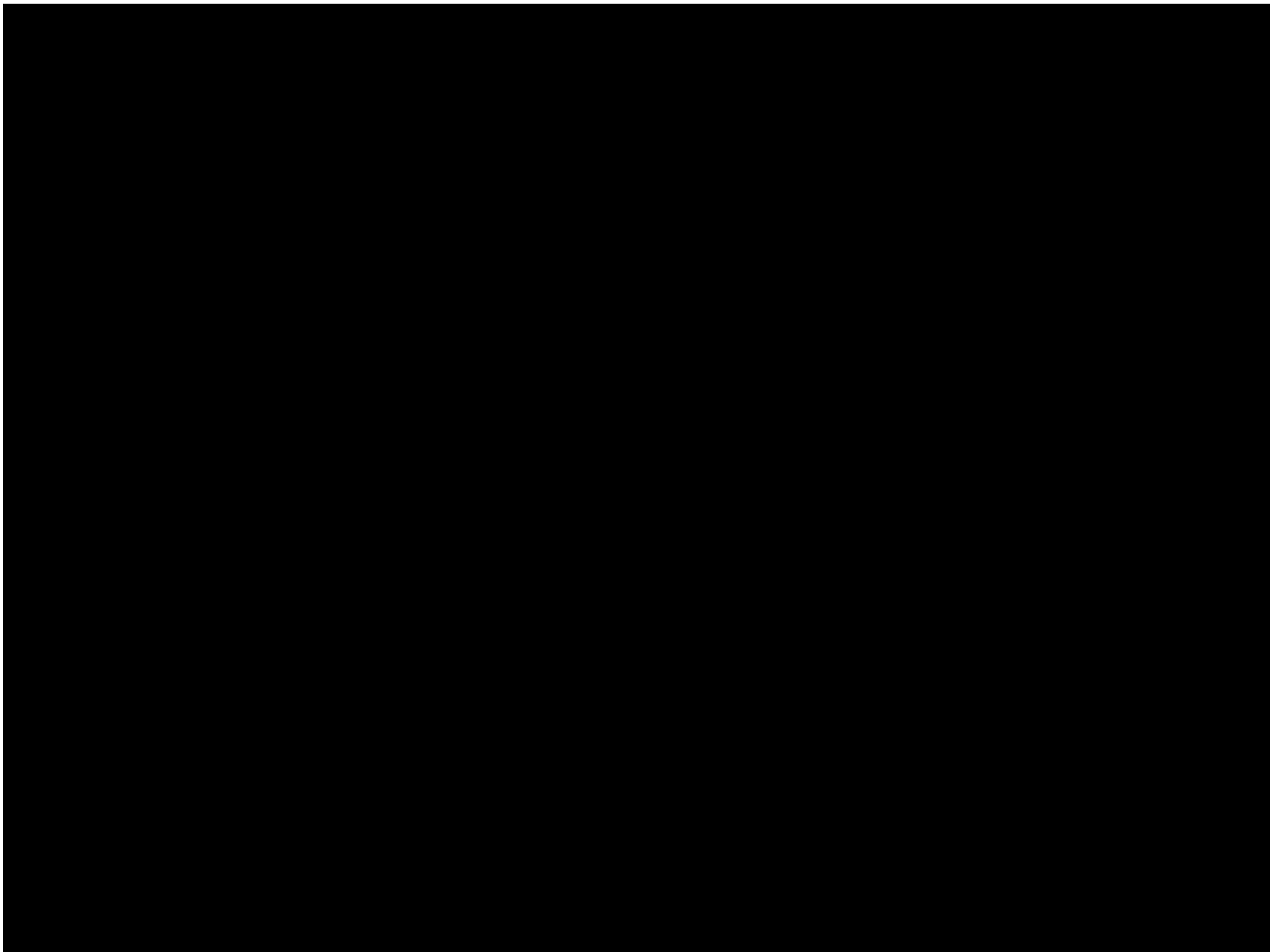
# Conclusions

All the **necessary ingredients are available** to realize declarative modeling languages for ML/DM

- machine learning & data mining
- declarative modeling and constraint programming
- programming language technology
- should work for unsupervised, clustering ... as well

So let's do it ...

Questions ?



What if we succeed?



# Our work today ...

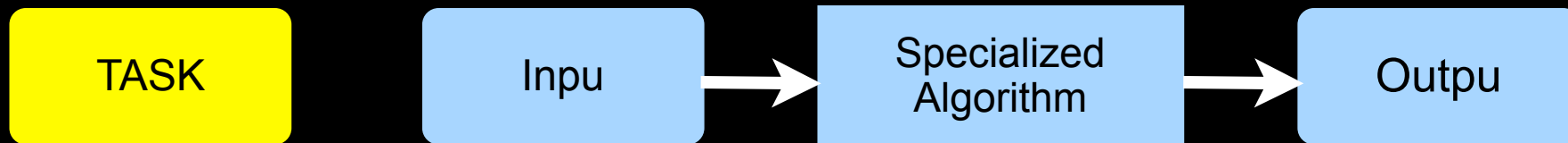
We typically have to

1. Formalize learning / mining task

2. Design algorithm / technique to use **Focus on**

3. Implement the algorithm **HOW** to **solve** problem

4. Use and distribute the software



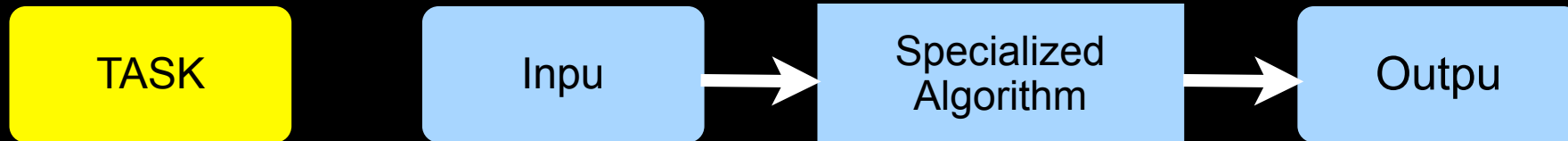
# Our work tomorrow ...

We typically have to

1. Formalize learning / mining task

2. Build a declarative mode More user perspective

4. Use and distribute the software

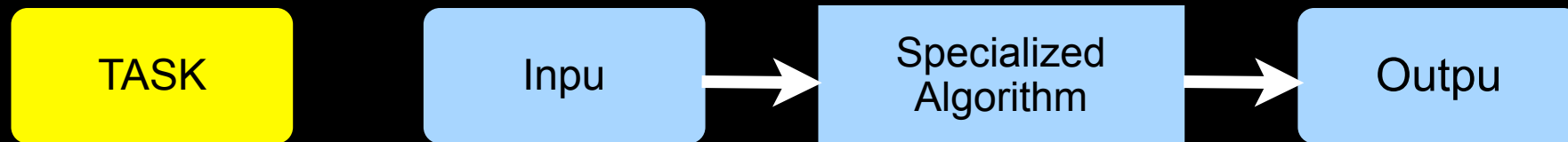


# Our work tomorrow ...

1. Work on Engines

2. Solvers translations ...

4. Use and distribute the software



# Our work tomorrow ?

Work on modeling

Theory ...

Work on translations

Work on solvers

Much more reuse of systems and techniques

Questions ?