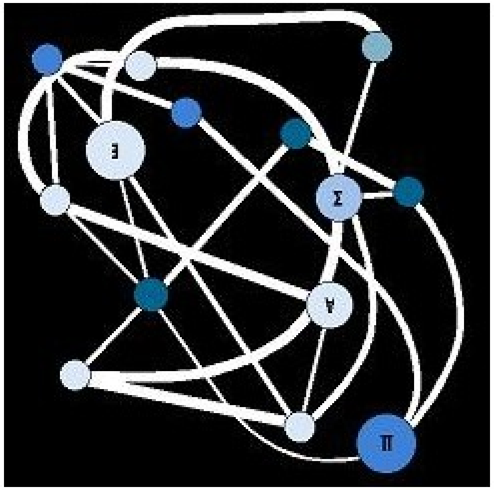
Relational Machine Learning



(Multi) Relational Data Mining

- Inductive Logic Programming (ILP)
- Probabilistic Reasoning – PR
- ILP + PR = SRL
- Statistical Relational Learning

Deductive Reasoning

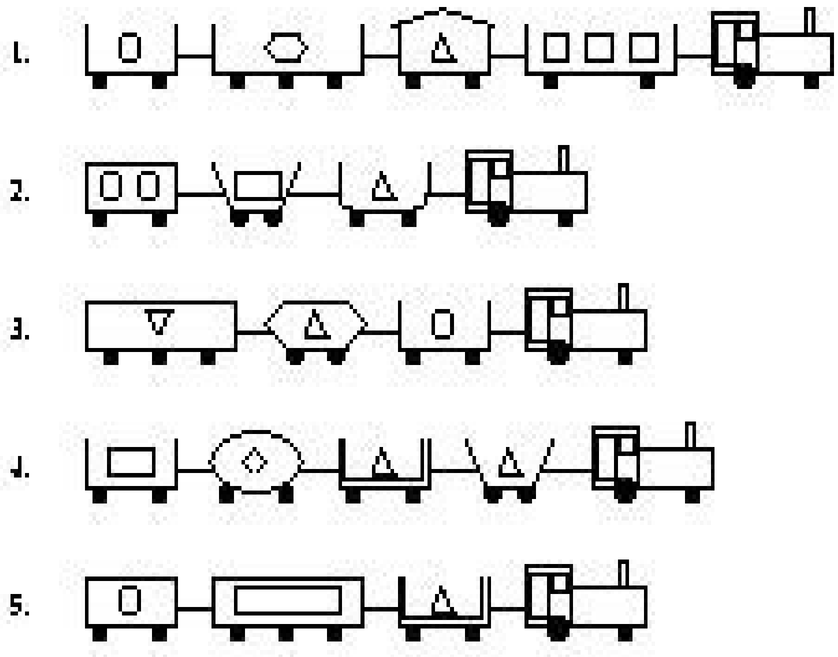
T ∪ B ⊨ E

T	∪	B	⊨	E
parent(X,Y) :- mother(X,Y) parent(X,Y) :- father(X,Y)	∪	mother(penelope,victoria) mother(penelope,artur) father(christopher,victoria) father(christopher,artur)	⊨	parent(penelope,victoria) parent(penelope,artur) parent(christopher,victoria) parent(christopher,artur)

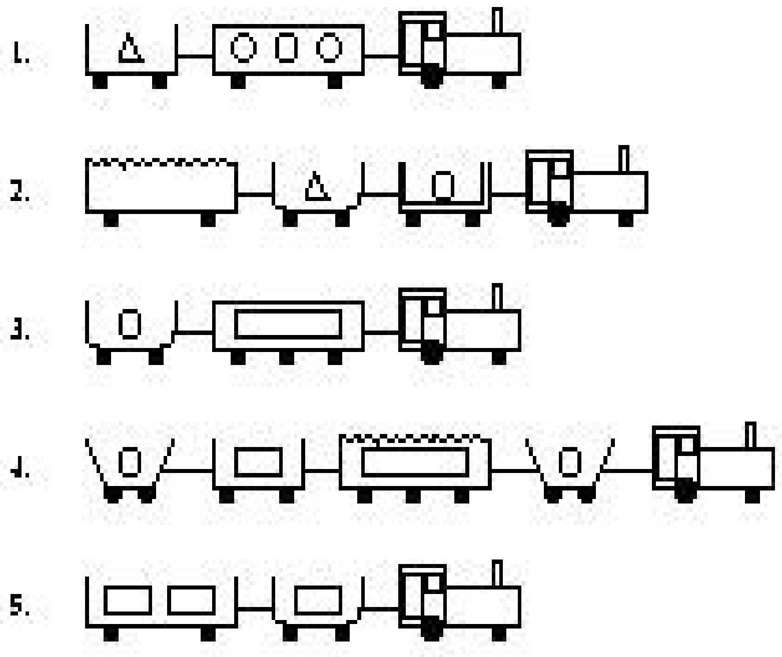
Inductive Reasoning

E	∪	B	⊨	T
parent(penelope,victoria) parent(penelope,artur) parent(christopher,victoria) parent(christopher,artur)	∪	mother(penelope,victoria) mother(penelope,artur) father(christopher,victoria) father(christopher,artur)	⊨	parent(X,Y) :- mother(X,Y) parent(X,Y) :- father(X,Y)

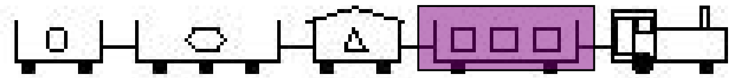
TRAINS GOING EAST



TRAINS GOING WEST



Inductive Logic Programming: example

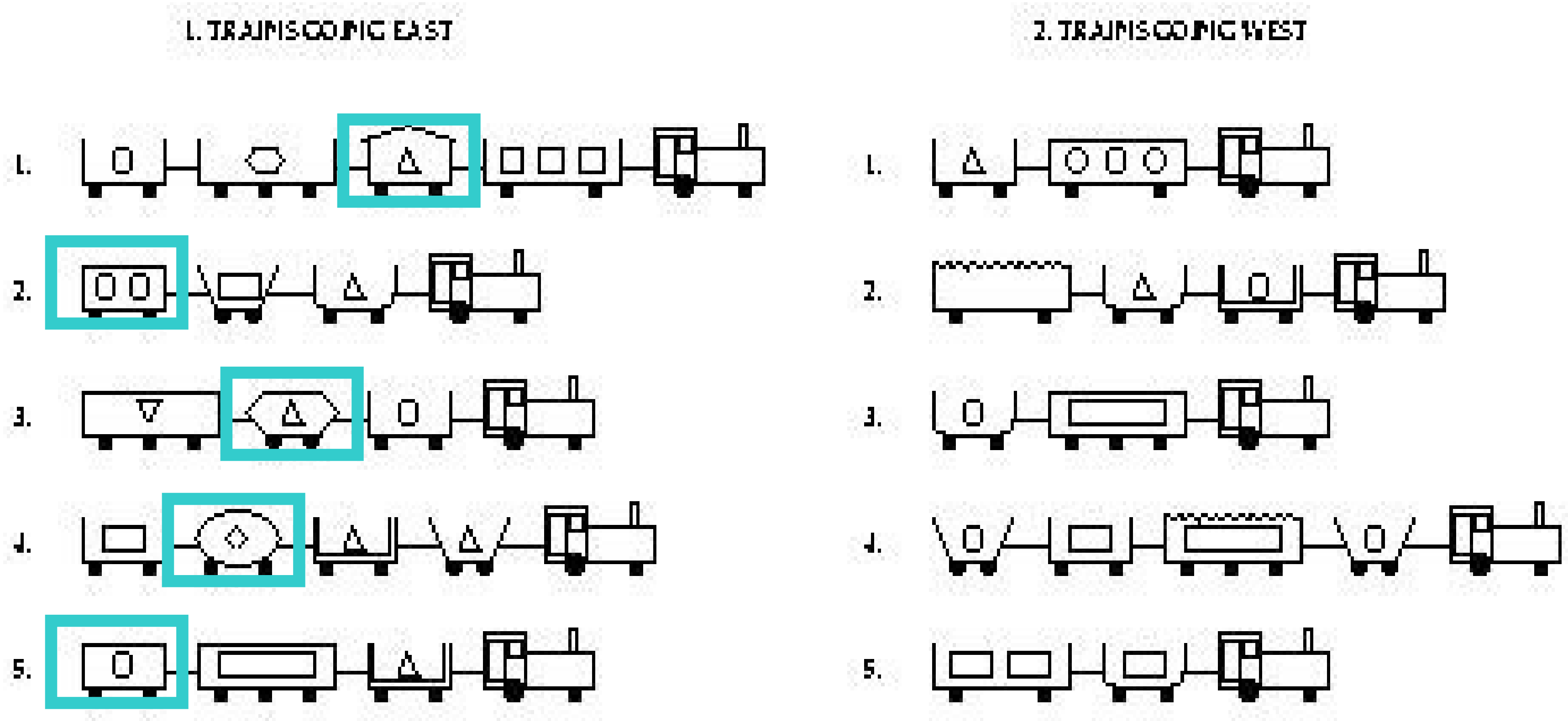


short(car_12).
closed(car_12).
long(car_11).
long(car_13).
short(car_14).
open_car(car_11).
open_car(car_13).
open_car(car_14).
shape(car_11,rectangle).
shape(car_12,rectangle).
shape(car_13,rectangle).
shape(car_14,rectangle).

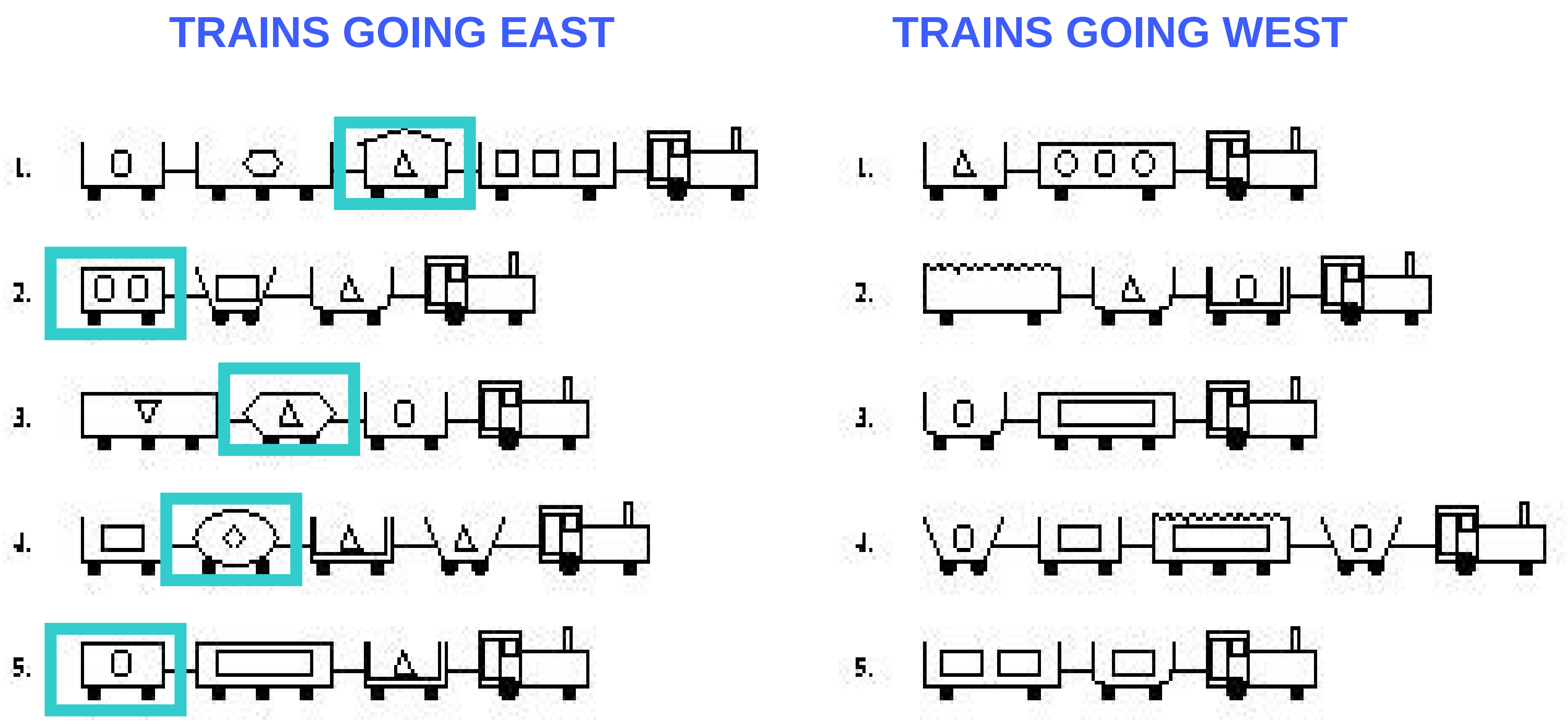
load(car_11,rectangle,3).
load(car_12,triangle,1).
load(car_13,hexagon,1).
load(car_14,circle,1).
wheels(car_11,2).
wheels(car_12,2).
wheels(car_13,3).
wheels(car_14,2).
has_car(east1,car_11).
has_car(east1,car_12).
has_car(east1,car_13).
has_car(east1,car_14).

Inductive Logic Programming: example

TRAINS GOING EAST **TRAINS GOING WEST**



Inductive Logic Programming: example



eastbound(T) IF has_car(T,C) AND short(C) AND closed(C)

Another example: extracting knowledge from mammogram annotations

```
is_malignant(A)  if
  'BIRADS_category'(A,b5),'MassPAO'(A,present),'Age'(A,age6570),
  previous_finding(A,B), 'MassesShape'(B,none),
  'Calc_Punctate'(B,notPresent),
  previous_finding(A,C), 'BIRADS_category'(C,b3) .
```

Esta regra diz que A é um caso maligno SE:

A is classified as BI-RADS 5 AND had a mass present
in a patient who:
  was between the ages of 65 and 70
  had two prior mammograms (B, C)
AND prior mammogram (B):
  had no mass shape described
  had no punctate calcifications
AND prior mammogram (C) was classified as BI-RADS 3

BI-RADS: **B**reast **I**maging **R**eporting **A**nd **D**ata **S**ystem

Inductive Logic Programming

- More formally:
- Given:
  - A set of examples **e** (observations, cases, instances) labelled as positive or negative (class **c**)
  - A language
  - Possibly, a set of constraints
- Find:
  - A hypothesis h, such that $\mathbf{h(e_i) = c_i}$
  - For most examples

Inductive Logic Programming

- Advantages:
  - Utilization of a language that is easy to interpret
  - More concise classifiers
  - More powerful representation: relations
- Disadvantages:
  - Very large search space
  - Non-probabilistic classification

Properties

- Prior satisfiability

$$B \wedge E^- \not\models \square$$

(H is not a consequence of B and E-)

- Posterior sufficiency

$$B \wedge H \models E^+$$

(H allows to explain E+ relative to B)

- Posterior satisfiability

$$B \wedge H \wedge E^- \not\models \square$$

(B and H are consistente with E-)

- Prior necessity

$$B \not\models E+$$

(some e+ must be false relative to the model found for B)

ILP: A Common Approach

- Use a greedy covering algorithm.
  - Repeat while some positive examples remain uncovered (not entailed):
    - Find a *good clause* (one that covers as many positive examples as possible but no/few negatives).
    - Add that clause to the current theory, and remove the positive examples that it covers.
- ILP algorithms use this approach but vary in their method for finding a *good clause*.

Some ILP Systems

- PROGOL, ALEPH (top-down): saturates first uncovered positive example, and then performs top-down admissible search of the lattice above this saturated example.
- GOLEM (bottom-up), FOIL (top-down), LINUS/DINUS.
- Tilde, Claudien, IndLog, ...

ILP Saturation

- Consists of building a *bottom clause* (seed)
- Incorporates background knowledge to an atomic formula
- Example: (gene that codes for a protein responsible for metabolism)

metabolism(A) :-
essential(A,'Non-Essential'), motif(A,'PS00510'), chromosome(A,'14'),
interaction(A,B,C,E),
essential(B,'Non-Essential'), motif(B,'PS00188'), chromosome(B,'2'),
interaction(A,F,D,G),
intertype(C,'Genetic'), intertype(D,?),
interaction(B,A,C,E),
interaction(B,H,C,I),
interaction(F,A,D,G),
interaction(H,B,C,I), interaction(H,_,_,_).

ILP: Aleph

- Procedure to extract theories from examples
- Complete (branch-and-bound) search for best clause in the ***whole*** space
- Search subject to several user control settings
  - Max clause length
  - Max chaining length
  - Minacc
  - Max nodes
  - Search strategy, etc.

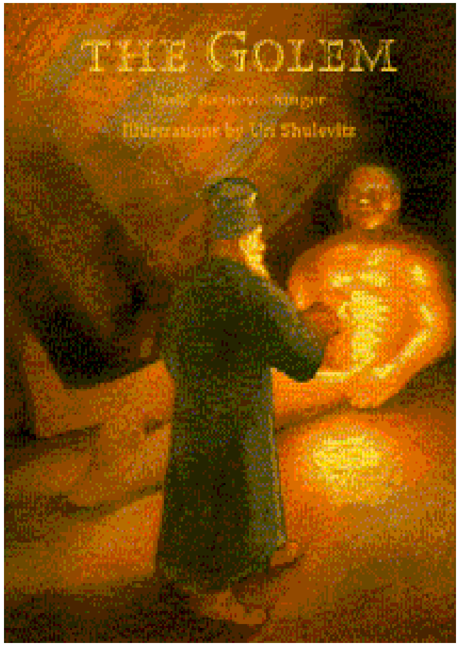
ILP: Aleph

- Aleph
  - Desenvolvido na Universidade de Oxford por Ashwin Srinivasan

http://www.comlab.ox.ac.uk/oucl/research/areas/machlearn/Aleph/

ILP: Aleph

Then the Rabbi said,
"*Golem, you have not been completely formed, but I am about to finish you now…You will do as I will tell you.*"
Saying these words, Rabbi Leib finished engraving the letter Aleph.
Immediately the golem began to rise.



Aleph: algorithm

- Initial State:
  - Examples or observations
  - Descriptions: background knowledge (BK)
- Final State: hypothesis or theory or model
- Transitions: intermediate hypotheses

Aleph: algorithm

- Select example
- Build most-specific-clause (**bottom clause**)
- Search. Find a clause more general than the bottom clause
- Remove redundant. The clause with the best score is added to the current theory, and all examples made redundant are removed. This step is sometimes called the "**cover removal**" step. Note here that the best clause may make clauses other than the examples redundant
- Return to first step

Aleph: Knowledge Representation

Input Files: Prolog Syntax

dtp.b: BK
dtp.f: pos examples
dtp.n: neg examples

Representation: BK

```
chromosome('G234064','1').
chromosome('G234065','1').
chromosome('G234070','1').
chromosome('G234073','1').
chromosome('G234074','1').
chromosome('G234076','1').
chromosome('G234084','2').
chromosome('G234085','2').
chromosome('G234089','2').
```

Representation: BK

interaction('G234062','G235011','Physical',?).
interaction('G234064','G234126','Genetic-Physical','0.9141').
interaction('G234064','G235065','Genetic-Physical','0.7515').
interaction('G234064','G235571','Physical','0.9691').
interaction('G234065','G234073','Physical','0.7492').
interaction('G234065','G235042','Physical','-0.4659').

Representation: Examples

metabolism('G239098').
metabolism('G234980').
metabolism('G235245').
metabolism('G234108').
metabolism('G238387').
metabolism('G240504').
metabolism('G236733').

Example of clause learned

metabolism(A) :-

chromosome(A,'15'),

interaction(A,B,_,_),

complex(B,'Transcription complexes/Transcriptosome').

A and *B* are variables that represent genes

Aleph: algorithm

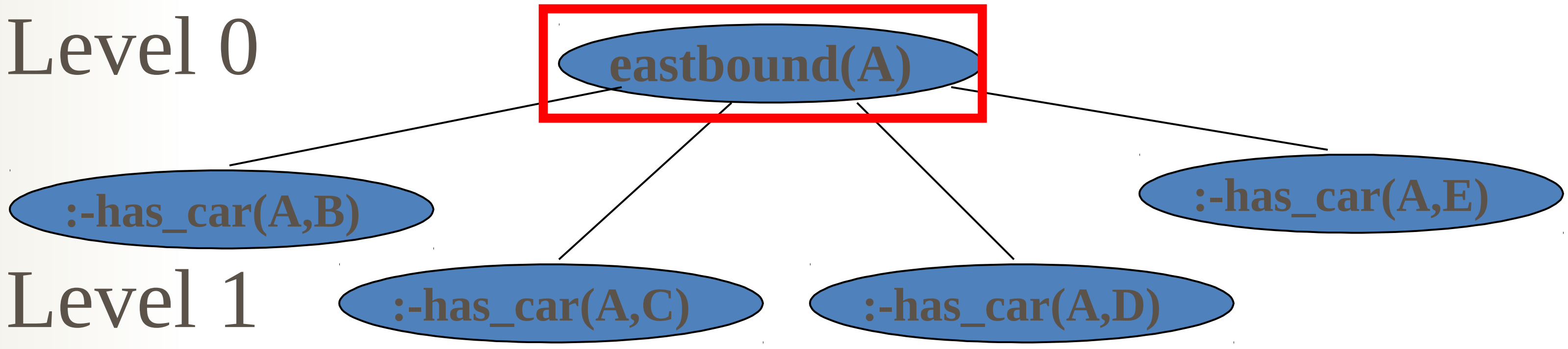
- Example: Michalski´s trains

Aleph: algorithm

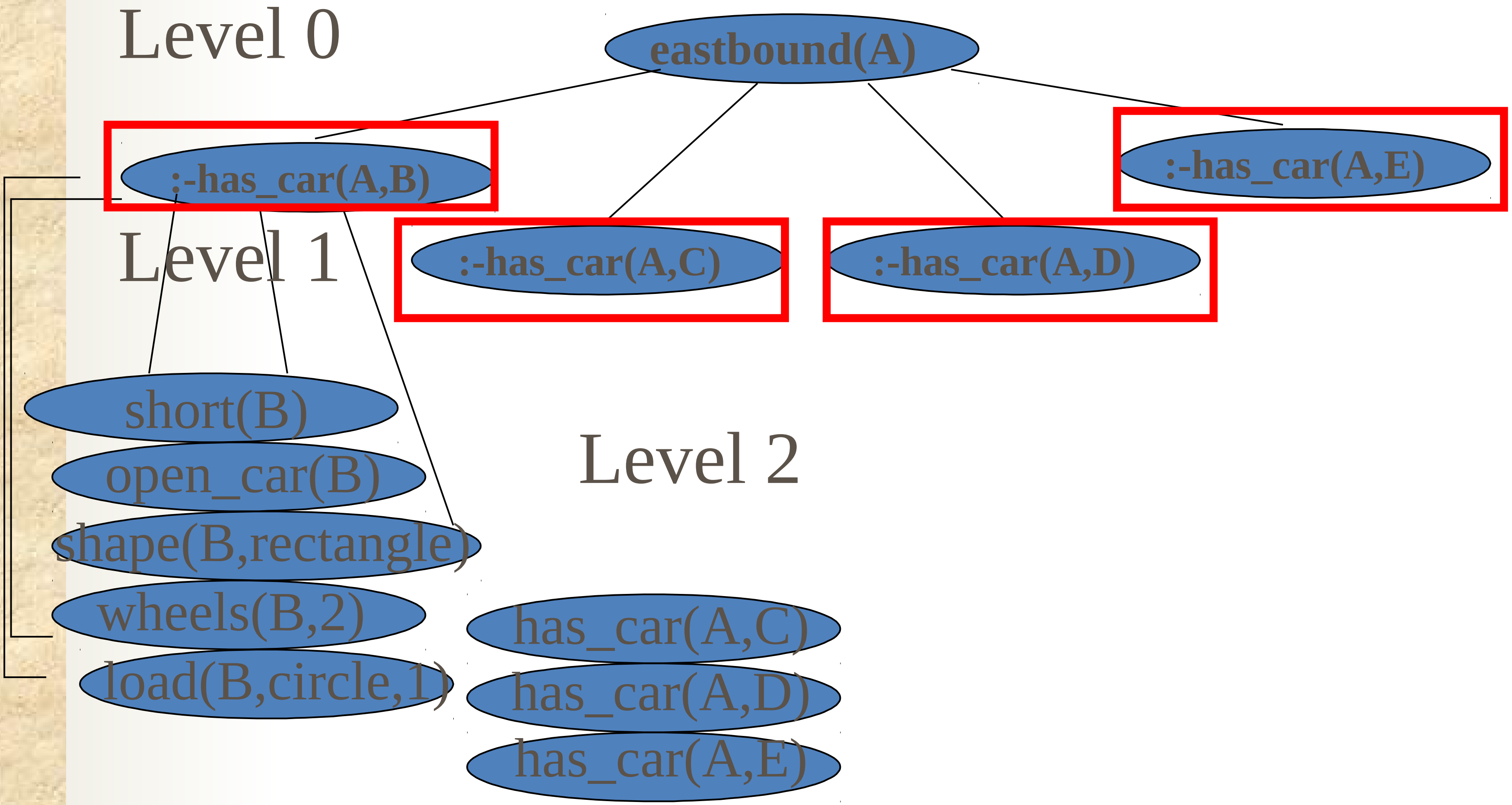
- Saturation (saturated / bottom clause):

eastbound(A) :-
has_car(A,B), has_car(A,C), has_car(A,D), has_car(A,E),
short(B), short(D), closed(D), long(C),
long(E), open_car(B), open_car(C), open_car(E),
shape(B,rectangle), shape(C,rectangle), shape(D,rectangle),
shape(E,rectangle),
wheels(B,2), wheels(C,3), wheels(D,2), wheels(E,2),
load(B,circle,1), load(C,hexagon,1), load(D,triangle,1),
load(E,rectangle,3).

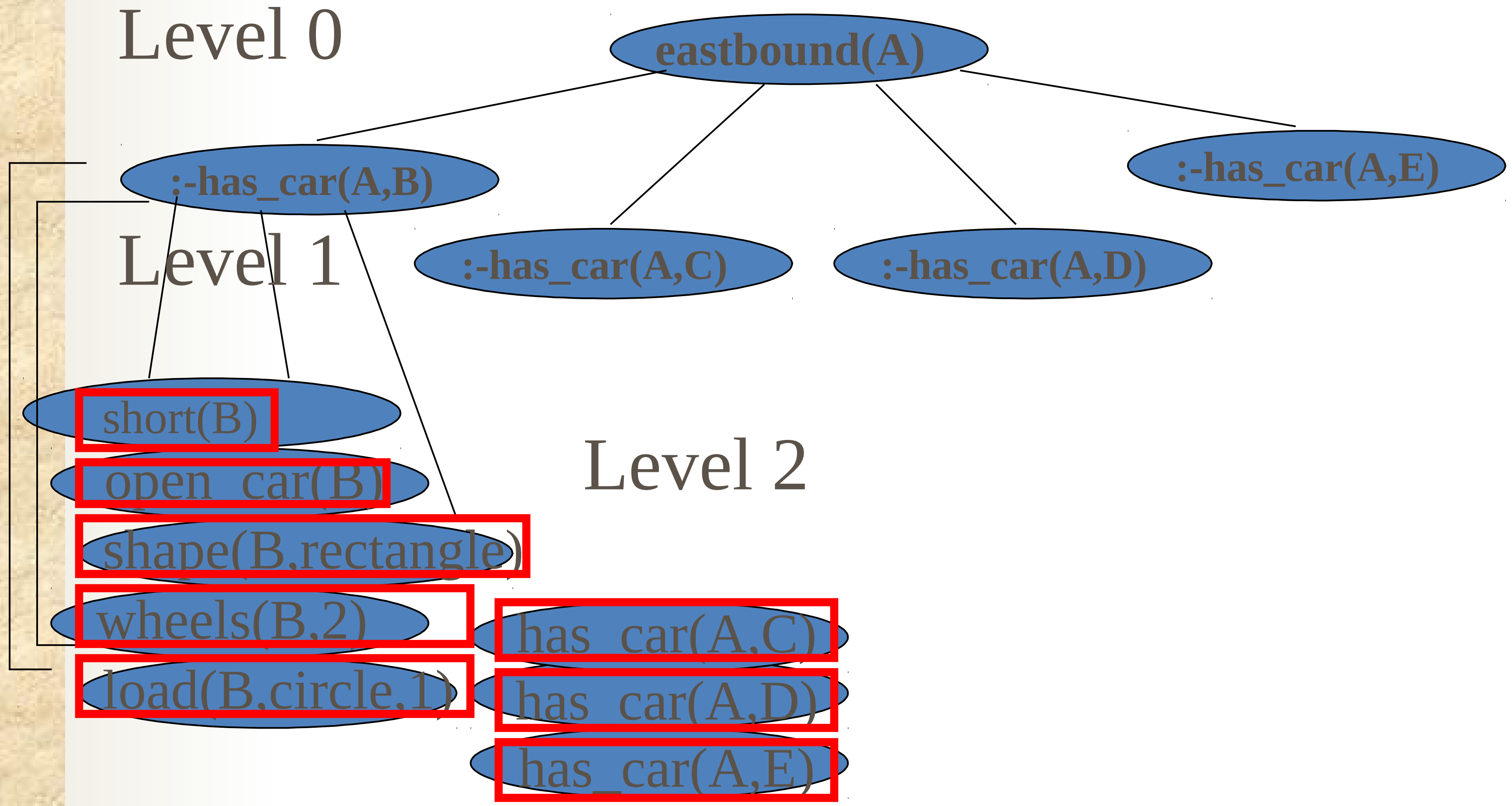
Aleph: Search



Aleph: Search



Aleph: Search



Aleph: algorithm

- Search: most general clause

eastbound(A) :-
has_car(A,B), has_car(A,C), has_car(A,D), has_car(A,E),
short(B), short(D), closed(D), long(C),
long(E), open_car(B), open_car(C), open_car(E),
shape(B,rectangle), shape(C,rectangle), shape(D,rectangle),
shape(E,rectangle),
wheels(B,2), wheels(C,3), wheels(D,2), wheels(E,2),
load(B,circle,1), load(C,hexagon,1), load(D,triangle,1),
load(E,rectangle,3).

Aleph: algorithm

- Search: add possible descendants (candidate literals of level 1)

eastbound(A) :-
has_car(A,B), has_car(A,C), has_car(A,D), has_car(A,E),
short(B), short(D), closed(D), long(C),
long(E), open_car(B), open_car(C), open_car(E),
shape(B,rectangle), shape(C,rectangle), shape(D,rectangle),
shape(E,rectangle),
wheels(B,2), wheels(C,3), wheels(D,2), wheels(E,2),
load(B,circle,1), load(C,hexagon,1), load(D,triangle,1),
load(E,rectangle,3).

Aleph: algorithm

- Search: add possible descendants of level 2

```
eastbound(A) :-
   has_car(A,B), has_car(A,C), has_car(A,D), has_car(A,E),
   short(B), short(D), closed(D), long(C),
   long(E), open_car(B), open_car(C), open_car(E),
   shape(B,rectangle), shape(C,rectangle), shape(D,rectangle),
   shape(E,rectangle),
   wheels(B,2), wheels(C,3), wheels(D,2), wheels(E,2),
   load(B,circle,1), load(C,hexagon,1), load(D,triangle,1),
   load(E,rectangle,3).
```

Aleph: algorithm

- Search: second descendant of level 1

eastbound(A) :-
has_car(A,B), has_car(A,C), has_car(A,D), has_car(A,E),
short(B), short(D), closed(D), long(C),
long(E), open_car(B), open_car(C), open_car(E),
shape(B,rectangle), shape(C,rectangle), shape(D,rectangle),
shape(E,rectangle),
wheels(B,2), wheels(C,3), wheels(D,2), wheels(E,2),
load(B,circle,1), load(C,hexagon,1), load(D,triangle,1),
load(E,rectangle,3).

Aleph: algorithm

- Search: descendants of second descendant…

```
eastbound(A) :-
  has_car(A,B), has_car(A,C), has_car(A,D), has_car(A,E),
  short(B), short(D), closed(D), long(C),
  long(E), open_car(B), open_car(C), open_car(E),
  shape(B,rectangle), shape(C,rectangle), shape(D,rectangle),
  shape(E,rectangle),
  wheels(B,2), wheels(C,3), wheels(D,2), wheels(E,2),
  load(B,circle,1), load(C,hexagon,1), load(D,triangle,1),
  load(E,rectangle,3).
```

Aleph: example of run

- aleph_trains

Aleph: how to run?

- You need to have a Prolog system
  - Yap: http://yap.sourceforge.net OR
  - SWI: http://www.**swi**-prolog.org
- Aleph: http://www.comlab.ox.ac.uk/oucl/research/areas/machlearn/Aleph/
- Files: .b, .f, .n
- To make things easier: everything in the same directory!

Aleph: Basic Commands

- read_all
- reduce
- induce

Aleph: Parameters

```
:- set(clauselength,5).
:- set(depth, 200).
:- set(i,3).
:- set(noise,0).
:- set(minacc,0.7).
:- set(nodes,1000000).
:- set(m,20).
:- set(evalfn,mestimate).
:- set(test_pos,'/u/dutra/Protein/prot_test_set.f').
:- set(test_neg,'/u/dutra/Protein/prot_test_set.n').
:- set(optimise_clauses,true).

:- set(record,true).
:- set(recordfile,'prot_train_set.out').
:- set(samplesize,0).
```

Strength estimate = (*support* + *m* * *prior*) / (*coverage* + *m*)

M → 0, strength → precision

Support = True positives

Coverage = True positives + false negatives

Aleph: Modes and Types

```
:- modeh(1,eastbound(+train)).
:- modeb(1,short(+car)).
:- modeb(1,closed(+car)).
:- modeb(1,long(+car)).
:- modeb(1,open_car(+car)).
:- modeb(1,double(+car)).
:- modeb(1,jagged(+car)).
:- modeb(1,shape(+car,#shape)).
:- modeb(1,load(+car,#shape,#int)).
:- modeb(1,wheels(+car,#int)).
:- modeb(*,has_car(+train,-car)).
```

```
:- determination(eastbound/1,short/1).
:- determination(eastbound/1,closed/1).
:- determination(eastbound/1,long/1).
:- determination(eastbound/1,open_car/1).
:- determination(eastbound/1,double/1).
:- determination(eastbound/1,jagged/1).
:- determination(eastbound/1,shape/2).
:- determination(eastbound/1,wheels/2).
:- determination(eastbound/1,has_car/2).
:- determination(eastbound/1,load/3).
```

Aleph: Modes and Types

```
:- modeh(1,metabolism(+gene)).

:- modeb(1,essential(+gene,#essential)).
:- modeb(1,class(+gene,#class)).
:- modeb(1,complex(+gene,#complex)).
:- modeb(1,phenotype(+gene,#phenotype)).
:- modeb(1,motif(+gene,#motif)).
:- modeb(1,chromosome(+gene,#chromosome)).
:- modeb(*,gte(+number,#number)).
:- modeb(*,interaction(+gene,-gene,-intertype,-number)).
:- modeb(1,intertype(+intertype,#intertype)).
```

Example: drug discovery using Aleph refinement operators

- Given:
  - Molecules active and inactive for dtp
  - Their description in terms of coordinates and bonds
- Find small structures that model active molecules

Examples: drug discovery

- Examples of dtp groups:

```
hydrophobic(m752,
        hyphob([a2, a3, a5, a8, a7, a4, a2],
        2.16452, -0.833917, 3.6379)).
hacc(m9706,
    hacc(a10, -6.2969, -1.3684, -0.4631)).
```

Example: drug discovery

- Utilisation of refinement operator

```
refine(false,Clause):-
   member(Point1, [hydrophobic(M,P1), hdonor(M,P1),halogen(M,P1),hacc(M,P1)]),
   member(Point2,[hydrophobic(M,P2),hdonor(M,P2),halogen(M,P2),hacc(M,P2)]),
   Clause = (active(M) :- Point1, Point2, dist(M,P1,P2,D1,E)).


refine(Clause1,Clause2):-
      Clause1 = (active(M) :- Point1,Point2, dist(M,P1,P2,D1,E)),      member(Point3,
      [hydrophobic(M,P3),hdonor(M,P3),halogen(M,P3),hacc(M,P3)]),
      Clause2 = (active(M) :- Point1, Point2, dist(M,P1,P2,D1,E),
                  Point3, dist(M,P1,P3,D2,E), dist(M,P2,P3,D3,E)).
```

- Reduce search space!!!

Exercises

- Basic Workshop:

http://www.dcc.fc.up.pt/~ines/aulas/1819/JISIC/ALEPH/aleph_workshop.html