

AUTOMATED REASONING

Agostino Dovier

Università di Udine
CLPLAB

Udine, November 2016

Modeling CSP with ASP

SUDOKU

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

SUDOKU

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

We want to define the predicate $x(\text{riga}, \text{colonna}, \text{valore})$

$x(1, 3, 1)$.

$x(2, 3, 2)$. $x(2, 5, 3)$. $x(2, 9, 4)$.

$x(3, 4, 5)$. $x(3, 7, 6)$. $x(3, 9, 7)$.

$x(4, 1, 5)$. $x(4, 4, 1)$. $x(4, 5, 2)$.

$x(5, 2, 7)$. $x(5, 8, 2)$.

$x(6, 5, 7)$. $x(6, 6, 8)$. $x(6, 9, 9)$.

$x(7, 1, 8)$. $x(7, 3, 7)$. $x(7, 6, 9)$.

$x(8, 1, 4)$. $x(8, 5, 6)$. $x(8, 7, 3)$.

$x(9, 7, 5)$.

SUDOKU

```
coord(1..9).
val(1..9).

% Assign a pair (X,Y) to a subsquare
square(I,X,Y) :-
    coord(X), coord(Y), coord(I),
    I == (X-1) / 3 + 3*((Y-1) / 3) + 1.

% x is a function
1 { x(X,Y,N) : val(N) } 1 :- coord(X), coord(Y).

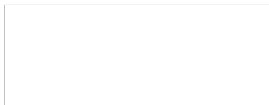
% x is injective on columns
1 { x(X,Y,N) : coord(X) } 1 :- coord(Y), val(N).

% x is injective on rows
1 { x(X,Y,N) : coord(Y) } 1 :- coord(X), val(N).

% x is injective in subsquares
1 { x(X,Y,N) : square(I,X,Y) } 1 :- val(N), coord(I).
```



Comitato Udinese Staffette Telethon



FONDAZIONE



```
slot(1..4). %%% cambia con 24
runner(X) :- can(X,_).
runner(X) :- ok(X,_).
available(X,T) :- can(X,T).
available(X,T) :- ok(X,T).

%% Biiezione runner/slot
1 { corrialle(X,T): slot(T) } 1 :- runner(X).
1 { corrialle(X,T): runner(X) } 1 :- slot(T).

%% Controllo disponibilita'
:- runner(X), slot(T), corrialle(X,T), not available(X,T).

%%% MINIMIZZIAMO GLI SLOT non OK
fastidio(F) :- F = #count{X : runner(X), slot(T), corrialle(X,T), not ok(X,T)}.
#minimize {F:fastidio(F)}.

#show corrialle/2.
#show fastidio/1.

%%% INPUT DATA, For each of the 24 player
%%% ok - good, can -maybe
can(ago,1). ok(ago,2). can(ago,3).
can(simone,1). can(simone,2). ok(simone,4).
ok(alberto,2). can(alberto,4).
can(fausto,1). can(fausto,4).
```

SOCCER TOURNAMENT



SOCCER TOURNAMENT

```
squadra(a;b;c;d; e;f;g;h) .  
giorno(1..7).    %% 1 lunedì', ..., 7 domenica  
feriale(1..5).  %%  
settimana(1..s) .  
orario(17;19;21) .  
  
slot(G,S,O)      :- giorno(G), settimana(S), orario(O) .  
squadreord(X,Y) :- squadra(X), squadra(Y), X < Y.
```

SOCCER TOURNAMENT

```
testaserie(a;b;c;d).
testeserie(A,B) :- testaserie(A),testaserie(B), A < B.

% Every pair of teams plays each other exactly once
1 { gioca(X,Y,G,S,O): slot(G,S,O) } 1 :- squadreord(X,Y).
% For each time slot, there is at most one match
0 { gioca(X,Y,G,S,O): squadreord(X,Y) } 1 :- slot(G,S,O).
```

Auxiliary Predicates:

```
oggi(X, S, X, S)           :- giorno(X), settimana(S).
domani(X, S, X+1, S)       :- giorno(X), giorno(X+1), settimana(S).
domani(7, S, 1, S+1)       :- settimana(S), settimana(S+1).
dopodomani(X, S, X+2, S)   :- giorno(X), giorno(X+2), settimana(S).
dopodomani(7, S, 2, S+1)   :- settimana(S), settimana(S+1).
dopodomani(6, S, 1, S+1)   :- settimana(S), settimana(S+1).
good(X1, S1, X2, S2) :-
    giorno(X1), giorno(X2),
    settimana(S1), settimana(S2),
    not oggi(X1, S1, X2, S2),
    not domani(X1, S1, X2, S2),
    not domani(X2, S2, X1, S1),
    not dopodomani(X1, S1, X2, S2),
    not dopodomani(X2, S2, X1, S1).
```

SOCCER TOURNAMENT

Constraints:

```
% At least three days between matches

:- squadreord(X,Y), squadreord(X,Z), Y < Z,
   slot(G1,S1,O1), slot(G2,S2,O2),
   gioca(X,Y,G1,S1,O1),gioca(X,Z,G2,S2,O2),
   not good(G1,S1,G2,S2).

:- squadreord(X,Y), squadreord(Z,X), Y != Z,
   slot(G1,S1,O1), slot(G2,S2,O2),
   gioca(X,Y,G1,S1,O1),gioca(Z,X,G2,S2,O2),
   not good(G1,S1,G2,S2).

:- squadreord(Y,X), squadreord(Z,X), Y < Z,
   slot(G1,S1,O1), slot(G2,S2,O2),
   gioca(Y,X,G1,S1,O1),gioca(Z,X,G2,S2,O2),
   not good(G1,S1,G2,S2).
```

SOCCER TOURNAMENT

Constraints:

```
% No matches Tue and Wed at 21.00 (there's champions league in TV)
:- squadreord(X,Y), settimana(S), gioca(X,Y,2,S,21).
:- squadreord(X,Y), settimana(S), gioca(X,Y,3,S,21).
% No matches Sat and Sun at 21.00 (there's the Serie A)
:- squadreord(X,Y), settimana(S), gioca(X,Y,6,S,21).
:- squadreord(X,Y), settimana(S), gioca(X,Y,7,S,21).

%%% best teams don't fight each other in the first week
:- testeserie(X,Y), slot(G,S,O), gioca(X,Y,G,S,O), S < 2.
%%% At most one match between best teams in the same day
:- testeserie(X1,X2), testeserie(X3,X4),
   slot(G,S,O1), slot(G,S,O2), O1 < O2,
   gioca(X1,X2,G,S,O1), gioca(X3,X4,G,S,O2).

%%% There are not working days without matches
slotoccupato(G,S,O) :-
   slot(G,S,O), squadreord(X,Y), gioca(X,Y,G,S,O).
giorno_occupato(G,S) :-
   slot(G,S,O), slotoccupato(G,S,O).
:- feriale(G), settimana(S), not giorno_occupato(G,S).
```

SOCCER TOURNAMENT

USING MINIMIZE

Constraints:

```
giorno_singolo(G,S) :-
    giorno(G), settimana(S), orario(O1), orario(O2), orario(O3),
    O1 != O2, O1 != O3, O2 < O3,
    slotoccupato(G,S,O1),
    not slotoccupato(G,S,O2),
    not slotoccupato(G,S,O3).

%%% If single match, it is at 19
:- giorno(G), settimana(S), giorno_singolo(G,S), slotoccupato(G,S,17).
:- giorno(G), settimana(S), giorno_singolo(G,S), slotoccupato(G,S,21).

%%% If two matches no hole inside
:- giorno(G), settimana(S), not giorno_singolo(G,S),
    slotoccupato(G,S,17), not slotoccupato(G,S,19), slotoccupato(G,S,21).

%%% MINIMIZE THE DAYS WITH SINGLE MATCH
contagiornisingoli(N) :- N = #count{G,S : giorno_singolo(G,S)}.
#minimize {N:contagiornisingoli(N)}.
```

SOCCER TOURNAMENT

“Special” constraints:

```
% The team "a" can't play on saturday
% (some players play basketball)
:- settimana(S), orario(O), squadra(Y), gioca(a,Y,6,S,O).
:- settimana(S), orario(O), squadra(Y), gioca(Y,a,6,S,O).
% The team "a" can't play on monday
% (some girlfriends close the shop)
:- settimana(S), orario(O), squadra(Y), gioca(b,Y,1,S,O).
:- settimana(S), orario(O), squadra(Y), gioca(Y,b,1,S,O).
% In the first and last day there must be at least 2 matches
:- orario(O1), orario(O2), O1 < O2,
   not slotoccupato(1,1,O1), not slotoccupato(1,1,O2).
:- orario(O1), orario(O2), O1 < O2,
   not slotoccupato(7,s,O1), not slotoccupato(7,s,O2).
```

Output predicates

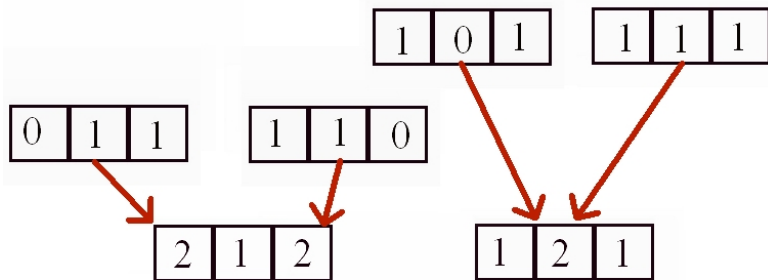
```
day(A, X1, X2, X3, X4, X5, X6) :-  
    giorno(G),  
    settimana(S),  
    A = G + 7*(S-1),  
    completamento(X1, X2, G, S, 17),  
    completamento(X3, X4, G, S, 19),  
    completamento(X5, X6, G, S, 21).  
completamento(X, Y, G, S, O) :-  
    slot(G, S, O), squadreord(X, Y), gioca(X, Y, G, S, O).  
completamento(nil, nil, G, S, O) :-  
    slot(G, S, O), not slotoccupato(G, S, O).
```


HAPLOTYPE INFERENCE

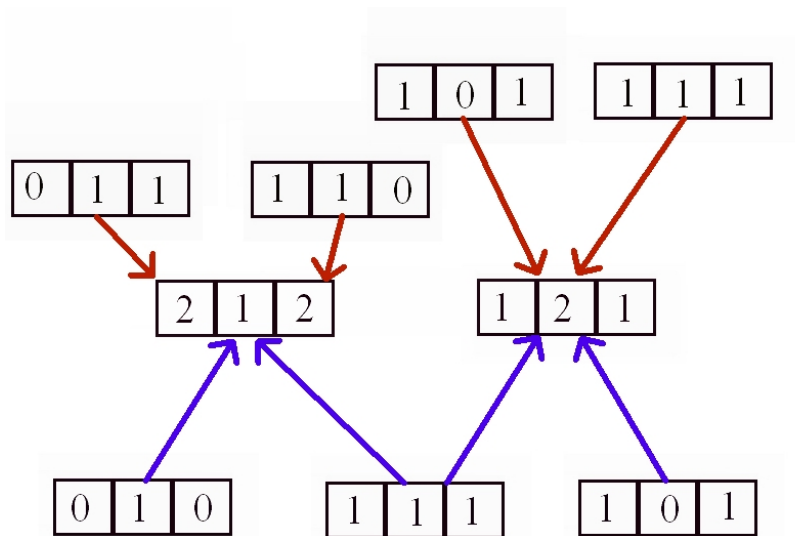
2	1	2
---	---	---

1	2	1
---	---	---

HAPLOTYPE INFERENCE



HAPLOTYPE INFERENCE



HAPLOTYPE INFERENCE

- Let $H \subseteq \{0, 1\}^n$ be a set of *haplotypes* and
- $G \subseteq \{0, 1, 2\}^n$ be a set of *genotypes*.
- Given $h_1, h_2 \in H$ and $g \in G$, $\{h_1, h_2\}$ **explains** g if and only if $|h_1| = |h_2| = |g|$ and $\forall i \in [1..n]$:

$$\begin{aligned}g[i] \leq 1 &\longrightarrow h_1[i] = h_2[i] = g[i] \\g[i] = 2 &\longrightarrow h_1[i] \neq h_2[i]\end{aligned}$$

- A set of haplotypes H explains a set of genotypes G if for all $g \in G$ there are $h_1, h_2 \in H$ such that $\{h_1, h_2\}$ explains g .
- Given a set of genotypes G and an integer k , the *haplotype inference problem (HIP)* **by pure parsimony** is the problem of finding a set H that explains G and such that $|H| = k$ (decision version: NP complete).

HAPLOTYPE INFERENCE

THE ASP MODELING

- m input genotypes ($1 \dots m$)
- $2m$ potential haplotypes ($1 \dots 2m$, not necessarily distinct)
- The i -th genotype g_i is explained by haplotypes h_{2i} and h_{2i-1}
- `geno(1..m) ., site(1..n) . and haplo(1..2m) .`
- Facts: `g(i, j, k) .` describes genotypes, where
 - i is the i -th genotype,
 - j is the position within the genotype and
 - k is the value in $\{0,1,2\}$
- `h(i, j) .` describe haplotypes.
It is in the model iff the value of the haplotype i at position j is 1

HAPLOTYPE INFERENCE

THE ASP MODELING

```
% If g(i,j)=0 or 1 assign deterministically
% h(2i) and h(2i-1).
(1)    h(2*I-1,J) :- g(I,J,1).
(2)    h(2*I,J)    :- g(I,J,1).
(3)    :- h(2*I-1,J), g(I,J,0).
(4)    :- h(2*I,J),   g(I,J,0).
% If g(i,j)=2 then exactly one between
% h(2i) and h(2i-1) is 1
(5)    h(2*I-1,J) :- g(I,J,2), not h(2*I,J).
(6)    h(2*I,J)   :- g(I,J,2), not h(2*I-1,J).
```

HAPLOTYPE INFERENCE

THE ASP MODELING

- ```
(7) representative_haplo(A) :-
 haplo(A), not cover_someone(A).
(8) cover_someone(B) :-
 haplo(A;B), A < B, samehaplo(A,B).
```

- Define the representatives.
- The lowest index haplotype of a set of equal ones is selected as representative.

- ```
(9)    { samehaplo(A,B) } :- haplo(A), haplo(B), A < B.  
(10)   :- samehaplo(A,B), haplo(A;B), A < B,  
        site(S), h(A,S), not h(B,S).  
(11)   :- samehaplo(A,B), haplo(A;B), A < B,  
        site(S), not h(A,S), h(B,S).
```

```
% Count the number of representative and minimize it
```

- ```
(12) diff_haplo(N) :-
 N = #count{ A:representative_haplo(A) }.
```

# HAPLOTYPE INFERENCE

## THE ASP MODELING

- ```
(7)    representative_haplo(A) :-  
        haplo(A), not cover_someone(A).  
(8)    cover_someone(B) :-  
        haplo(A;B), A < B, samehaplo(A,B).  
(9)    { samehaplo(A,B) } :- haplo(A), haplo(B), A < B.  
(10)   :- samehaplo(A,B), haplo(A;B), A < B,  
        site(S), h(A,S), not h(B,S).  
(11)   :- samehaplo(A,B), haplo(A;B), A < B,  
        site(S), not h(A,S), h(B,S).
```

- We have a (possibly empty) set of `samehaplo`.
- Constraints: can't be `samehaplo` and a site `S` with \neq values.
- `not (_, S)` for the case haplotype at site `S` is 0.
- Symmetry breaking.

```
% Count the number of representative and minimize it
```

```
(12) diff_haplo(N) :-
```


HAPLOTYPE INFERENCE

THE ASP MODELING

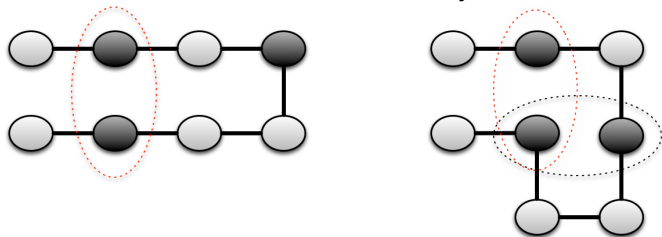
- ```
(7) representative_haplo(A) :-
 haplo(A), not cover_someone(A).
(8) cover_someone(B) :-
 haplo(A;B), A < B, samehaplo(A,B).
(9) { samehaplo(A,B) } :- haplo(A), haplo(B), A < B.
(10) :- samehaplo(A,B), haplo(A;B), A < B,
 site(S), h(A,S), not h(B,S).
(11) :- samehaplo(A,B), haplo(A;B), A < B,
 site(S), not h(A,S), h(B,S).

% Count the number of representative and minimize it
(12) diff_haplo(N) :-
 N = #count{ A:representative_haplo(A) }.
(13) #minimize{ N:diff_haplo(N)}.
```

# THE PROTEIN STRUCTURE PREDICTION PROBLEM

## MODEL

- The input is a list  $S$  of amino acids  $S = s_1, \dots, s_n$ ,
- where  $s_i \in \{h, p\}$
- Each  $s_i$  is placed on a 2D grid with integer coordinates
- Any pair of two amino acids can't occupy the same position
- If two amino acids are at distance 1, they are in **contact**



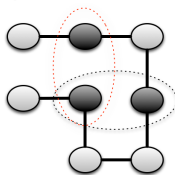
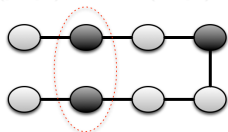
# THE PROTEIN STRUCTURE PREDICTION PROBLEM

## MODEL

- A folding is a function  $\omega : \{1, \dots, n\} \rightarrow \mathbb{N}^2$  where
- $\forall i \text{ next}(\omega(i), \omega(i+1))$  and
- $\forall i, j (i \neq j \rightarrow \omega(i) \neq \omega(j))$
- $\text{next}(\langle X_1, Y_1 \rangle, \langle X_2, Y_2 \rangle) \iff |X_1 - X_2| + |Y_1 - Y_2| = 1.$
- Find a folding that minimizes the (simplified) energy function:

$$E(S, \omega) = \sum_{\substack{1 \leq i \leq n-2 \\ i+2 \leq j \leq n}} \text{Pot}(s_i, s_j) \cdot \text{next}(\omega(i), \omega(j))$$

where  $\text{Pot}(p, p) = \text{Pot}(h, p) = \text{Pot}(p, h) = 0$  and  $\text{Pot}(h, h) = -1.$



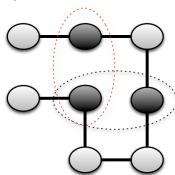
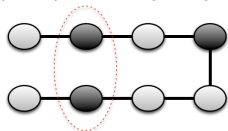
# THE PROTEIN STRUCTURE PREDICTION PROBLEM

## MODEL

- A folding is a function  $\omega : \{1, \dots, n\} \rightarrow \mathbb{N}^2$  where
- $\forall i \text{ next}(\omega(i), \omega(i+1))$  and
- $\forall i, j (i \neq j \rightarrow \omega(i) \neq \omega(j))$
- $\text{next}(\langle X_1, Y_1 \rangle, \langle X_2, Y_2 \rangle) \iff |X_1 - X_2| + |Y_1 - Y_2| = 1.$
- Find a folding that minimizes the (simplified) energy function:

$$E(S, \omega) = \sum_{\substack{1 \leq i \leq n-2 \\ i+2 \leq j \leq n}} \text{Pot}(s_i, s_j) \cdot \text{next}(\omega(i), \omega(j))$$

where  $\text{Pot}(p, p) = \text{Pot}(h, p) = \text{Pot}(p, h) = 0$  and  $\text{Pot}(h, h) = -1.$



# THE PROTEIN STRUCTURE PREDICTION PROBLEM

## ASP MODEL

- The positions can be restricted to  $[1 \dots 2n] \times [1 \dots 2n]$
- The first two amino acids are set to  $\omega(1) = \langle n, n \rangle$  and  $\omega(2) = \langle n, n + 1 \rangle$
- Sequence is represented by  $n$  facts:

```
prot(1,p). prot(2,h). prot(3,p). prot(4,h).
prot(5,p). prot(6,p). prot(7,h). prot(8,p).
```

- Each placement is stored as `sol(i,X,Y)`.

# ASP ENCODING

```
(1) size(N) :- N = #count{ I:prot(I,J) }.
(2) board(1..2*N) :- size(N).
(3) range(X,Y) :- size(N), board(X;Y),
 |X-N| < N , |Y-N| < N.
```

- Count the protein length and defines the board size
- range is loaded with all combinations from 1 to 2N

```
(4) sol(1,N,N) :- size(N).
(5) sol(2,N,N+1) :- size(N).

(6) 1 { sol(I,X,Y) : range(X,Y) } 1 :- prot(I,Amino).

(7) :- prot(I1,A1), prot(I2,A2), I1<I2,
 sol(I1,X,Y), sol(I2,X,Y), range(X,Y).
```

- (1) `size(N) :- N = #count{ I:prot(I,J) }.`
- (2) `board(1..2*N) :- size(N).`
- (3) `range(X,Y) :- size(N), board(X;Y),  
|X-N| < N , |Y-N| < N.`
- (4) `sol(1,N,N) :- size(N).`
- (5) `sol(2,N,N+1) :- size(N).`

- Set the first two amino acids positions

- (6) `1 { sol(I,X,Y) : range(X,Y) } 1 :- prot(I,Amino).`
- (7) `:- prot(I1,A1), prot(I2,A2), I1<I2,  
sol(I1,X,Y), sol(I2,X,Y), range(X,Y).`

- ```
(1) size(N)          :- N = #count{ I:prot(I,J) }.
(2) board(1..2*N)   :- size(N).
(3) range(X,Y)      :- size(N), board(X;Y),
                       |X-N| < N , |Y-N| < N.

(4) sol(1,N,N)      :- size(N).
(5) sol(2,N,N+1)    :- size(N).

(6) 1 { sol(I,X,Y) : range(X,Y) } 1 :- prot(I,Amino).
```

- Each amino acid I is associated to a unique position

- ```
(7) :- prot(I1,A1), prot(I2,A2), I1<I2,
 sol(I1,X,Y), sol(I2,X,Y), range(X,Y).
```



- ```
(1) size(N)          :- N = #count{ I:prot(I,J) }.
(2) board(1..2*N)   :- size(N).
(3) range(X,Y)      :- size(N), board(X;Y),
                       |X-N| < N , |Y-N| < N.

(4) sol(1,N,N)      :- size(N).
(5) sol(2,N,N+1)    :- size(N).

(6) 1 { sol(I,X,Y) : range(X,Y) } 1 :- prot(I,Amino).

(7) :- prot(I1,A1), prot(I2,A2), I1<I2,
       sol(I1,X,Y), sol(I2,X,Y), range(X,Y).
```

- Constraint: two distinct amino acids can't overlap

```
(8) :- prot(I1,A1), prot(I2,A2), I2>1,  
      I1==I2-1, not next(I1,I2).  
(9)  next(I1,I2) :- prot(I1,A1), prot(I2,A2), I1<I2,  
      sol(I1,X1,Y1), sol(I2,X2,Y2),  
      range(X1,Y1), range(X2,Y2),  
      1 == |X2-X1| + |Y2-Y1|.
```

- Constraint: two consecutive amino acids in sequence are next in space

```
(10) energy_pair(I1,I2) :- prot(I1,h), prot(I2,h),  
      next(I1,I2), I1+2<I2,  
      1==(I2-I1) \ 2. %%% "\" is "mod"  
(11) energy(N) :- N = #count{(I1,I2):energy_pair(I1,I2)}.  
(12) #maximize { N:energy(N)}.
```

```
(8) :- prot(I1,A1), prot(I2,A2), I2>1,  
      I1==I2-1, not next(I1,I2).  
(9)  next(I1,I2) :- prot(I1,A1), prot(I2,A2), I1<I2,  
      sol(I1,X1,Y1), sol(I2,X2,Y2),  
      range(X1,Y1), range(X2,Y2),  
      1 == |X2-X1| + |Y2-Y1|.   
  
(10) energy_pair(I1,I2) :- prot(I1,h), prot(I2,h),  
      next(I1,I2), I1+2<I2,  
      1==(I2-I1) \ 2. %%% "\" is "mod"  
(11) energy(N) :- N = #count{ (I1,I2):energy_pair(I1,I2) }.  
(12) #maximize { N:energy(N) }.
```

- If two amino acids of type h are `next`, count one contact (`energy_pair`)
- Optimization: at least one amino acid in sequence between the pair
- Optimization: only odd distances in space can contribute to a contact