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## Optimization in Graphical Models

Thomas Schiex

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# Optimization in Graphical Models

## Connecting NP-complete frameworks

T. Schiex, MIAT, INRA

Many more co-workers and contributors, see bibliography



November 2015 - ICTAI - Vietri sul Mare

## Powering numerous AI areas (several industry related)

- 1 Model Based Diagnosis, Planning,...
- 2 Scheduling, Configuration, Resource Allocation,...
- 3 NLP, Planning/reasoning under uncertainty (\*MDP)...

## Powering computer (and other) science areas

- 1 Verification, Cryptography, Testing
- 2 Image analysis (stereovision, segmentation...)
- 3 Statistics, Bioinformatics (structural biology)...

Various exact approaches: (weighted) SAT & CSP, ILP, QP...

## Informal

- ① A set of discrete variables, each with a domain
- ② We want to define a joint function on all those variables
- ③ We do this by combining small functions involving few variables

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## Why Graphical ?

- 1 a vertex per variable, a (hyper)edge per function
- 2 Or its incidence graph (Factor graphs<sup>28</sup>)
- 3 Allows to describe knowledge on a lot of variables concisely
- 4 Usually hard to manipulate (NP-hard queries).

## Constraint Network

- 1 Set  $X \ni x_i$  of  $n$  variables, with finite domain  $D^i$  ( $|D^i| \leq d$ )
- 2 Set  $C \ni c_S : D^S \rightarrow \{0, 1\}$  of  $e$  constraints
- 3  $c_S$  has scope  $S \subset X$  ( $|S| \leq r$ )
- 4 Defines a **factorized** joint constraint over  $X$ :

$$\forall t \in D^X, C(t) = \max_{c_S \in C} c_S(t[S])$$

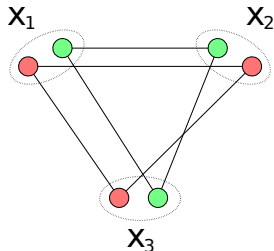
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## Graph coloring/RLFAP-feas

- 1 A graph  $G = (V, E)$  and  $m$  colors.
- 2 Can we color all vertices in such a way that no edge connects two vertices of the same color ?



## SAT

- 1 Variables  $x_i$  are boolean ( $0 \equiv \text{true}$ ,  $1 \equiv \text{false}$ )
- 2 Constraints are defined as clauses  $l_{i_1} \vee \dots \vee l_{i_p}$   
 $l_i$  is  $x_i$  or  $\bar{x}_i = (1 - x_i)$  (negation).
- 3 Truth value:  $(l_{i_1} \vee \dots \vee l_{i_p}) = l_{i_1} \times \dots \times l_{i_p}$

$$\forall t \in D^X, C(t) = \max_{c_S \in C} c_S(t[S])$$



Simply

Shift from boolean functions to cost functions

## Cost Function Networks - Weighted Constraint Networks

- Variables and domains as usual
- Cost functions  $W \ni c_S : D^S \rightarrow \{0, \dots, k\}$  ( $k$  finite or not)
- Cost combined by (bounded) addition<sup>8</sup> (other, see VCSP<sup>46</sup>).

$$\text{cost}(t) = \sum_{c_S \in C} c_S(t[S]) \quad c_\emptyset : \text{lower bound}$$

A solution has cost  $< k$ . Optimal if minimum cost.

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## Benefits

- Defines feasibility and cost homogeneously
- A constraint is a cost function with costs in  $\{0, k\}$

- Just associate a positive integer cost  $v_i$  to each clause.
- Cost value:  $(l_{i_1} \vee \dots \vee l_{i_p}, v_i) = v_i \times (l_{i_1} \times \dots \times l_{i_p})$
- Minimize the sum of all these.
- Polynomial Pseudo-Boolean Optimization.<sup>5</sup>
- A clause with cost  $k$  is hard.

## Markov Random Fields, Bayesian Networks

- Random variables  $X$  with discrete domains
- joint probability distribution  $p(X)$  defined through the product of positive real-valued functions:

$$p(X = t) \propto \prod_{c_S \in \mathcal{C}} c_S(t[S])$$

Massively used in 2/3D Image Analysis, Statistical Physics, NLP, planning/reasoning under uncertainty. . .

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## Maximum a Posteriori MAP-MRF

MRF  $\equiv$  CFN up to a  $(-\log)$  transform.

## 01 LP Variables, for a binary MRF/CFN

- ①  $x_{ia}$ : value  $a$  used for variable  $x_i$ .
- ②  $y_{iajb}$ : pair  $(a, b)$  used for  $x_i$  and  $x_j$

$$\text{Minimize } \sum_{i,a} c_i(a) \cdot x_{ia} + \sum_{\substack{c_{ij} \in C \\ a \in D^i, b \in D^j}} c_{ij}(a, b) \cdot y_{iajb} \quad \text{subject to}$$

$$\sum_{a \in D^i} x_{ia} = 1 \quad \forall i \in \{1, \dots, n\}$$

$$\sum_{b \in D^j} y_{iajb} = x_{ia} \quad \forall c_{ij} \in C, \forall a \in D^i$$

$$x_{ia}, y_{iajb} \in \{0, 1\}$$

Linear relaxation : the local polytope<sup>47,25,53</sup>

## Exact approaches (beyond ILP)

- 1 Full dynamic programming (Variable elimination, <sup>3,13</sup> resolution<sup>12,43,14</sup>)
- 2 Tree search + fast, incremental approximate local reasoning

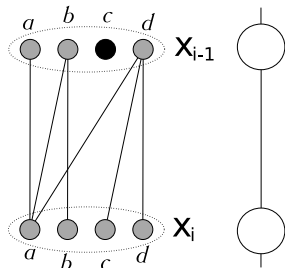
## Fast, approximate reasoning with some guarantees

- Arc Consistency and Unit Propagation (CSP/SAT)
- Message Passing (MRF/BN)
- Soft Arc Consistency in CFN and UP in PWMaxSAT



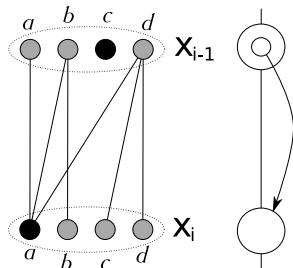
## AC as Dynamic programming

- Imagine a CSP with linear graph
- Which values of  $x_i$  belong to a solution of  $x_1, \dots, x_i$  knowing those for  $x_{i-1}$ .
- $\min_{x_{i-1}} (\max(c_{i-1}, c_{i,i-1}))$



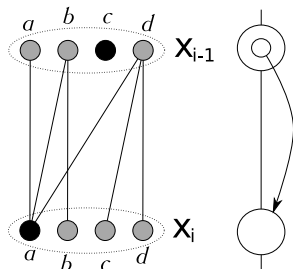
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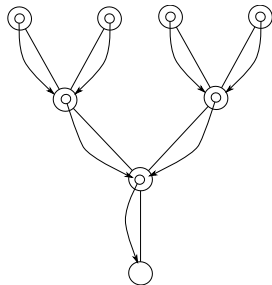


## Revise = Equivalence Preserving Transformation (EPT)

- $\nexists b \in D^j \mid c_{ij}(a, b) = 0$ .
- we can delete  $a$  in  $c_i$  (or  $D^i$ ).
- the resulting problem is equivalent (same set of solutions)

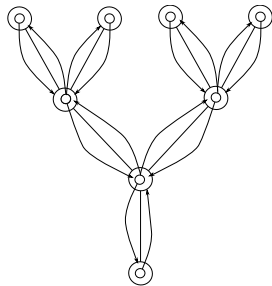
## Rooted tree CN

- Revise from leaves to root
- Root domain: values that belong to a solution



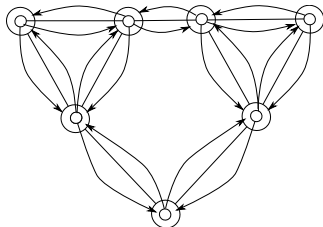
## Tree CN

- Revise from leaves and back
- All domains: values that belong to a solution
- Resulting problem solved backtrack-free<sup>20,19</sup>



## Arc consistency (Waltz 72)

- 1 Linear time (tables)
- 2 Unique fixpoint (confluent)
- 3 Preserves equivalence
- 4 May detect infeasibility
- 5 Problem transformation (incremental)



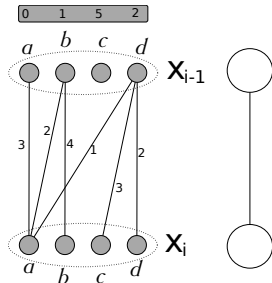
Maintaining AC during search.

- 1 Same update equation.
- 2 One literal and one clause.
- 3  $\min_{x_{i-1}}(\max(c_{i-1}, c_{i,i-1}))$

Maintaining UP during search (DPLL, ancestor of CDCL)

MP - Dynamic Programming<sup>40,28</sup>

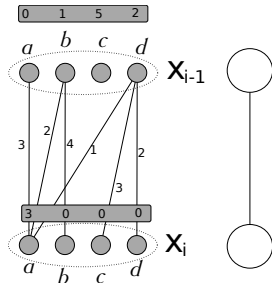
- 1 optimum cost from  $x_1$  to  $a \in D_i$  knowing those for  $x_{i-1}$
- 2  $\min_{x_{i-1}} (c_{i-1} + c_{i,i-1})$
- 3 Use external functions (messages) to store DP results





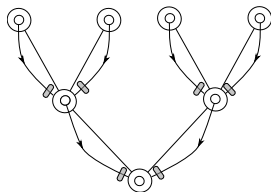
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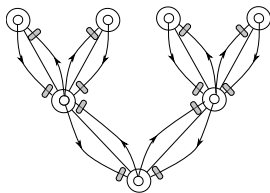
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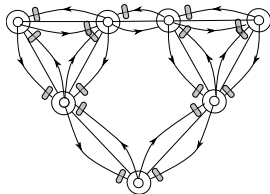
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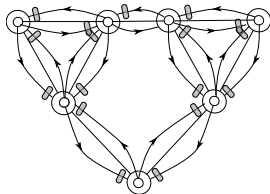
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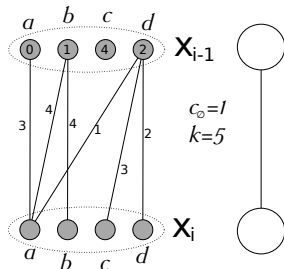
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- 1 Solves Berge acyclic MRF/BN (acyclic Factor Graphs)
- 2 Does not converge on graphs (Loopy Belief Propagation)
- 3 Massively used to produce “good” solutions (turbo-decoding<sup>42</sup>)
- 4 More recently introduced in Distributed COP<sup>18</sup>
- 5 Not an equivalence preserving transformation<sup>40</sup>

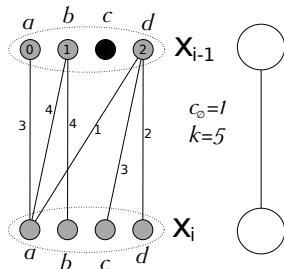
## Soft AC as Dynamic programming

- 1 MRF message passing but...
- 2 use  $c_\emptyset$  and  $c_i(\cdot)$  to store optimum cost from  $x_1$  to  $x_i$
- 3 Preserves equivalence by “cost shifting”<sup>47,52,45</sup>



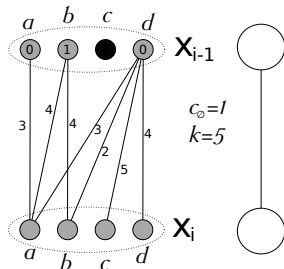
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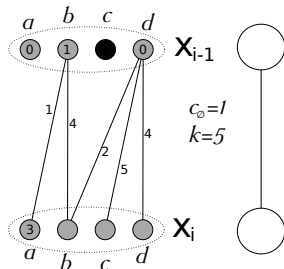
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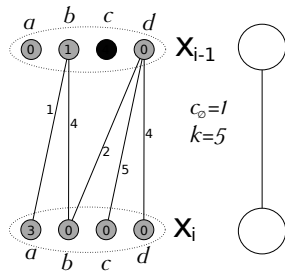
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Arc EPT: Project ( $\{ij\}, \{i\}, a, \alpha$ )

- Shifts  $\alpha$  units of cost between  $c_i(a)$  and  $c_{ij}$ .
- Shift direction: sign of  $\alpha$ .
- $\alpha$  constrained: no negative costs!

Precondition:  $-c_i(a) \leq \alpha \leq \min_{t' \in D^{ij}, t'[i]=a} c_{ij}(t')$ ;

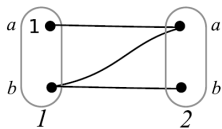
**Procedure** Project ( $\{i, j\}, \{i\}, a, \alpha$ )

$c_i(a) \leftarrow c_i(a) + \alpha$ ;

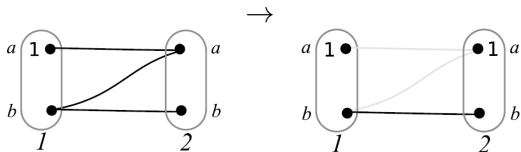
**foreach** ( $t' \in D^{ij}$  such that  $t'[i] = a, c_{ij}(t') < k$ ) **do**

$c_{ij}(t') \leftarrow c_{ij}(t') - \alpha$ ;

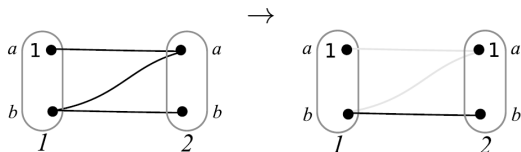
**end**



Project  $(\{1, 2\}, \{2\}, a, 1)$



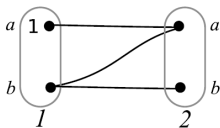
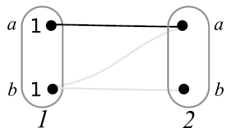
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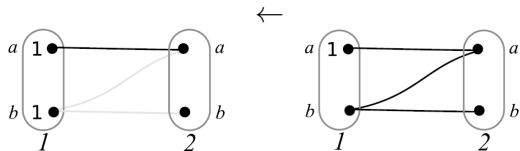
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$\text{Project}(\{1, 2\}, \{2\}, a, -1)$

Project  $(\{1, 2\}, \{1\}, b, 1)$



$\text{Project}(\{1, 2\}, \{1\}, b, 1)$

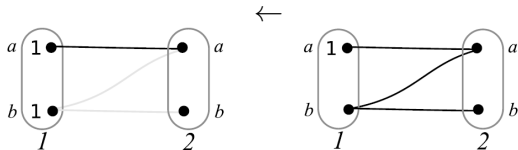


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$\text{Project}(\{1, 2\}, \{1\}, b, -1)$

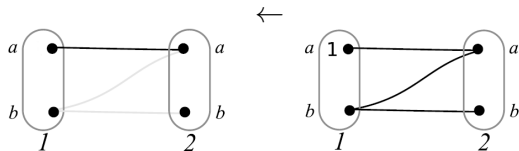


Project  $(\{1, 2\}, \{1\}, b, 1)$



$\Downarrow$  Project  $(\{1\}, \emptyset, [], 1)$

$\text{Project}(\{1, 2\}, \{1\}, b, 1)$



$\Downarrow \text{Project}(\{1\}, \emptyset, [], 1)$

$$c_{\emptyset} = 1$$

- Solves tree structured problems (ordering), optimum in  $c_{\emptyset}$
- Reformulation: incremental
- May loop indefinitely (graphs)
- No unique fixpoint (when it exists)
- Exploited since the 70s by the Ukrainian school<sup>47,27,26,53</sup> and for a subclass of ILP.<sup>52</sup>

## Breaking the loops

- 1 Arc consistency: prevent loops at the arc level<sup>45</sup>
- 2 Node consistency<sup>30</sup>
- 3 Directional AC: prevent loops at a global level<sup>6,32,33</sup>
- 4 Combine AC and DAC into FDAC<sup>32,33</sup>
- 5 Pool costs from all stars to  $c_{\emptyset}$  in EAC<sup>34</sup>
- 6 Combine AC+DAC+EAC in EDAC<sup>34</sup>

All  $O(ed)$  space. Equivalent to their “CSP” counterpart on constraints.

Semantically, it's the the same

- Problems with leftovers after cost shifting
- Includes non CNF (Heras, Larrosa<sup>31</sup>)
- Represented as a linear number of “compensation clauses”<sup>4</sup>

Finding an optimal order<sup>8</sup>

Finding an optimal sequence of integer arc EPTs that maximizes the lower bound is NP-hard.

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Finding an optimal sequence of integer arc EPTs that maximizes the lower bound is NP-hard.

Finding an optimal set<sup>7</sup>

Finding an optimal *set* of *rational* arc EPTs that maximizes the lower bound is in P.

This is achieved by solving an LP (OSAC, finite costs,  $k = \infty$ ).

## LP Variables, for a binary CFN

- 1  $u_i$ : amount of cost shifted from  $c_i$  to  $c_\emptyset$
- 2  $p_{ija}$ : amount of cost shifted from  $c_{ij}$  to  $a \in D^i$



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### OSAC

$$\begin{aligned}
 &\text{Maximize } \sum_{i=1}^n u_i && \text{subject to} \\
 &c_i(a) - u_i + \sum_{(c_{ij} \in C)} p_{ija} \geq 0 && \forall i \in \{1, \dots, n\}, \forall a \in D^i \\
 &c_{ij}(a, b) - p_{ija} - p_{jib} \geq 0 && \forall c_{ij} \in C, \forall (a, b) \in D^{ij}
 \end{aligned}$$

See [47, 25, 7, 53, 11].

## 01 LP Variables, for a binary CFN

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## The MRF local polytope<sup>53</sup>

$$\text{Minimize } \sum_{i,a} c_i(a) \cdot x_{ia} + \sum_{\substack{c_{ij} \in C \\ a \in D^i, b \in D^j}} c_{ij}(a, b) \cdot y_{iajb} \quad \text{s.t}$$

$$\sum_{a \in D^i} x_{ia} = 1 \quad \forall i \in \{1, \dots, n\} \quad (1)$$

$$\sum_{b \in D^j} y_{iajb} - x_{ia} = 0 \quad \forall c_{ij}/c_{ji} \in C, \forall a \in D^i \quad (2)$$

$u_i$  multiplier for (1) and  $p_{ija}$  for (2).

- ① Soft ACs (MP with reformulation) are approximate greedy Block Coordinate Descent solvers of the dual LP (OSAC).
- ② They find feasible (but non necessarily optimal) solutions of the dual.
- ③ optimal does not mean more efficient for tree search.

2015

Prusa and Werner<sup>41</sup> showed that any “normal” LP can be reduced to such a polytope in linear time (constructive proof).

Could soft arc consistency/MP speed-up LP?

$\text{Bool}(P)^{10}$

Given a CFN  $P = (X, D, C, k)$

$\text{Bool}(P)$  is the CSP  $(X, D, C - \{c_\emptyset\}, 1)$ .

$\text{Bool}(P)$  forbids all positive cost assignments, ignoring  $c_\emptyset$ .

## Bool( $P$ )<sup>10</sup>

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## Virtual AC

A CFN  $P$  is Virtual AC iff Bool( $P$ ) has a non empty AC closure.

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## Virtual AC

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## Virtual AC and MP

TRW-S,<sup>24</sup> MPLP1,<sup>49</sup> SRMP,<sup>23</sup> Max-Sum diffusion,<sup>27,11</sup> Aug-DAG<sup>26</sup>  
converge to fixpoints that satisfy the same property.

Solutions of  $\text{Bool}(P)$  are optimal in  $P$ .



Solutions of  $\text{Bool}(P)$  are optimal in  $P$ .

## VAC

- 1 solves tree-structured problems,
- 2 solves CFNs with submodular cost functions (Monge matrices)
- 3 solves CFNs for which AC is a decision procedure in  $\text{Bool}(P)$ .
- 4 if  $P$  is VAC and one value  $a$  in each domain such that  $c_i(a) = 0$  is solved.
- 5 There is always at least one such value (or else not VAC).

# In practice - Solvers

toulbar2, daoopt, AbsCons (Depth first tree search)

MaxHS, wpm1, wpm2, akmaxsat, minimaxsat. . . (DFS)

ILP-Cplex, QP-Cplex, SDP-BiqMac (Best first tree search)

OpenGM2 (MRF algorithms, Message passing and more).

CELAR 06,  $n = 100$ ,  $d = 44$  - one core

- 1 1997: 26 days of a Sun UltraSparc 167 MHz.
- 2 2015: optimum found in 7", proved in 73" (2.1GHz CPU)

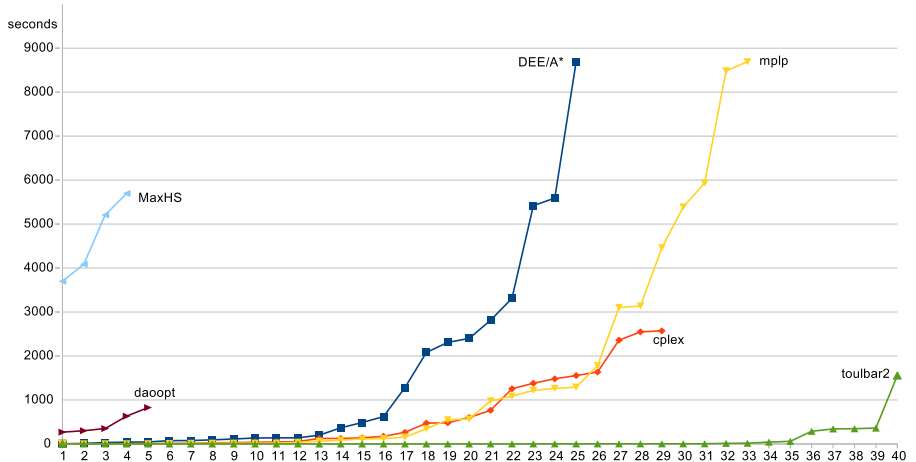
- 12.5 fold increase in frequency (+architecture)
- More than 30,000 times faster (now easy problem).
- All min-interference CELAR instances closed (see [fap.zib.de](http://fap.zib.de))

Design new enzymes for biofuels, drugs. . . cosmetics too

- Reduced to a non convex mixed optimization problem
- Discretized (non convexity) leading to a NP-hard. . .
- binary MAP-MRF capturing molecule stability based on atom-scale forces (electrostatics. . .)

- Few variables (from 10 to few hundreds)
- Huge domains (typ.  $d = 450$ )
- Exact solvers:  $A^*$ +substituability (DEE<sup>15</sup>), ILP<sup>22</sup>
- By far most used: simulated annealing (Rosetta<sup>21</sup>).

# Multi-paradigm comparison - QP,SDP,ILP,WMaxsat,MRF,CFN



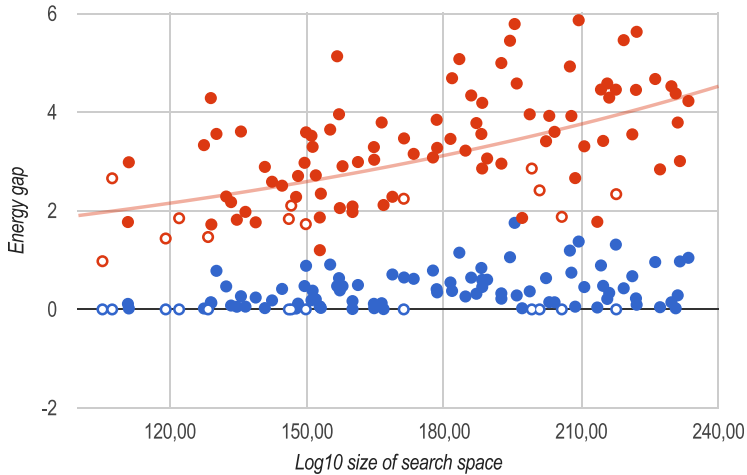
## CPLEX V12.4.0.0

```
Problem '3e4h.LP' read.  
Root relaxation solution time = 811.28 sec.  
...  
MIP - Integer optimal solution: Objective = 150023297067  
Solution time = 864.39 sec.
```

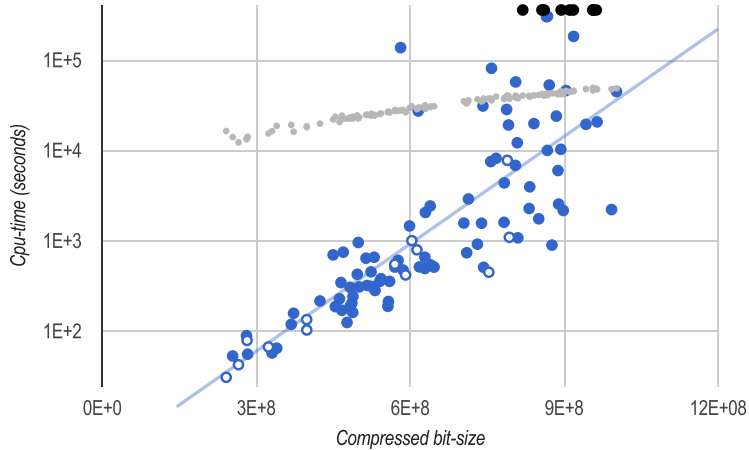
## tb2 and VAC

```
loading CFN file: 3e4h.wcsp  
Lb after VAC: 150023297067  
Preprocessing time: 9.13 seconds.  
Optimum: 150023297067 in 129 backtracks, 129 nodes and 9.38 seconds.
```

# Exact (simulated annealing is stochastic)<sup>48</sup>



# Faster than dedicated simulated annealing<sup>48</sup>





- ① First/second in approximate graphical model MRF/MAP challenges (2010, 2012, 2014).
- ② Global cost functions (weighted Regular, AllDiff, GCC...)
- ③ Bioinformatics: pedigree debugging,<sup>44</sup> Haplotyping (QTLMap), structured RNA gene finding<sup>54</sup>
- ④ Inductive Logic Programming,<sup>2</sup> Natural Language Processing (in hlt-di-13), Multi-agent and cost-based planning,<sup>29,9</sup> Model Abstraction,<sup>50</sup> diagnostic,<sup>36</sup> Music processing and Markov Logic,<sup>39,38</sup> Data mining,<sup>37</sup> Partially observable Markov Decision Processes,<sup>16</sup> Probabilistic counting<sup>17</sup> and inference,<sup>35</sup> ...

Everything is connected :-)

Questions ?



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