Optimization in Graphical Models - NP-complete optimization and its applications

Thomas Schiex

Optimization in Graphical Models

NP-complete optimization and its applications

T. Schiex

Many co-workers and contributors, see bibliography

AFIA General assembly
EurAI Fellowship
October 2016

The second era of AI

Spring of AI

- AI algorithms win chess championship, Deep Blue II, 1997.
- Computing power, RAM, search and a bit of ML (evaluation function)

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New Spring of AI

- Mostly computing power, ML and data.
- Before that, NP-hard problem solving (CP, SAT, search) has been providing major contributions to AI, in its theory and applications.

The power of NP-hard problem solving

Inside AI and computer science

1. Model Based Diagnosis, Planning,...
2. Scheduling, Configuration, Resource Allocation,...
3. Verification, Cryptography, Testing

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SAT, CSP, CP, ASP: satisfiability/feasibility

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Finding perfect solutions to perfectly defined problems

The world is often more complex
ML gives us the capacity to build models of complex systems from data.

Perfect solution to perfect problems

Early planning for GPS navigation

- A digital model of roads
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- Static model of reality
- Exact and efficient algorithm to decide from this “exact” model

Modern planning for GPS navigation

- Data on travel time on each road, at all time
- Feeds a stochastic model of duration
- Planning by minimizing expected time
- GPS navigation monitors plan execution

From data to decisions: **data analytics**

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Data analytics: what do we need ?

- Massive data
- A family of (stochastic) models that can be learnt
- On which optimization algorithms may apply
- Minimum requirement: efficient/tight bounds.

Definition

1. Set $X = \{x_1, \cdots, x_n\}$ of variables, each with a domain D^i
2. Set Φ of functions φ_S involving variables of $S \subset X$ (scope).
3. A joint function on X, $\mathbf{x} \in D^X$:

$$F(\mathbf{x}) = \bigoplus_{\varphi_S \in \Phi} \varphi_S(\mathbf{x}_S)$$

Graphical Model

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Why Graphical ?

1. a vertex per variable
2. an edge when 2 variables interact in a $\varphi_S \in \Phi$
3. Allows to describe knowledge on a lot of variables concisely
4. Usually hard to manipulate (NP-hard queries).

A Constraint Network is a graphical model

Constraint Network

1. Variables and domains
2. φ_S are Boolean functions (constraints, $\mathrm{t} \equiv 0 < 1 \equiv \mathrm{f}$)
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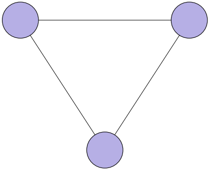
Graph coloring/RLFAP-feas

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 ?



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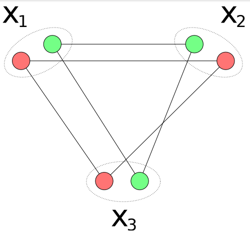

Beyond feasibility... optimization

Biology has very few general laws

Need to shift from perfect knowledge processing to approximate/imperfect knowledge processing

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Valued CSP

Shift from a conjunction of boolean functions to a more general combination of functions with a totally ordered co-domain (preferences, costs, priorities...)

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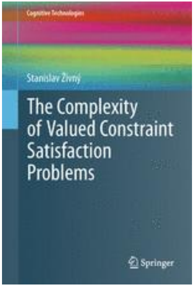

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Additive functions

Cost Function Networks - Weighted Constraint Networks - GAI models

- Variables and domains as usual
- Cost functions $\varphi_S : D^S \to \{0, \ldots, k\}$ (k finite or not)
- Combined by bounded addition[8]

$$F(\mathbf{x}) = \sum_{\varphi_S \in \Phi} \varphi_S(\mathbf{x}[S]) \qquad \varphi_\varnothing : \text{lower bound}$$

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 range $\{0, k\}$ only

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:

$$\mathsf{p}(\mathsf{X} = \mathbf{x}) \propto \prod_{\varphi_{\mathsf{S}} \in \Phi} \varphi_{\mathsf{S}}(\mathbf{x}_{\mathsf{S}})$$

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

Stochastic Graphical Models

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Maximum a Posteriori MAP-MRF

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

Binary CFN/MRF as 01LP

1. No constraint or determinism: infinite k, finite costs
2. v_{ia}: value a used for variable x_i.
3. p_{iajb}: pair (a, b) used for x_i and x_j

$$\text{Minimize} \sum_{i,a} \varphi_i(a) \cdot v_{ia} + \sum_{\substack{\varphi_{ij} \in \Phi \\ a \in D^i, b \in D^j}} \varphi_{ij}(a,b) \cdot p_{iajb} \quad \text{subject to}$$

$$\sum_{a \in D^i} v_{ia} = 1 \qquad \forall i \in \{1, \ldots, n\}$$

$$\sum_{b \in D^j} p_{iajb} = v_{ia} \qquad \forall \varphi_{ij} \in \Phi, \forall a \in D^i$$

$$v_{ia}, p_{iajb} \in \{0, 1\}$$

Continuous relaxation : the local polytope[45,25,54]

Exact approaches (beyond ILP)

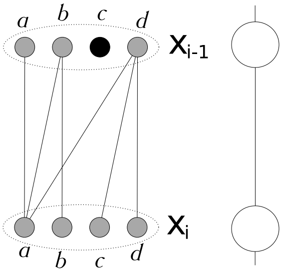
1. Dynamic programming (Variable and join-tree elimination,[2,12] resolution[11,40,13])
2. Tree search + fast, incremental approximate local reasoning (CP, SAT)

Fast, approximate reasoning with some guarantees

- Arc Consistency in CSP/CP
- Message Passing (MRF/BN)
- Soft Arc Consistency in CFN

AC as Dynamic programming

- Imagine a CSP with a linear graph
- Assume we know which values of D^{i-1} belongs to a solution on $x_1 \dots x_{i-1}$
- We can extend this to D^i for $x_1 \dots x_i$
- Let $f_i = \min_{x_{i-1}}(\max(\varphi_{i-1}, \varphi_{i,i-1}))$
- Include f_i in the problem



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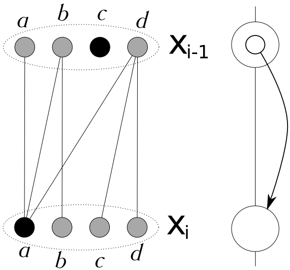

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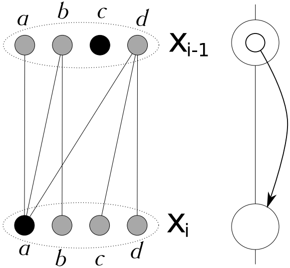


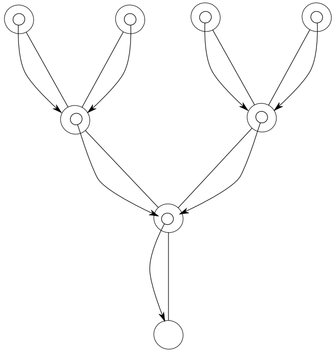
Revise: Equivalence Preserving Transformation

The resulting problem is equivalent (same set of solutions)

(Directional) AC solves Berge-acyclic CN

Rooted tree CN

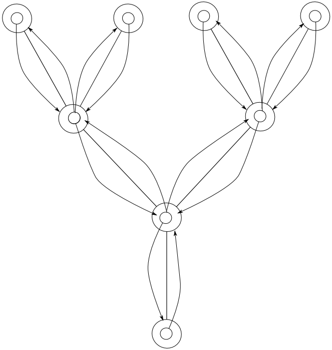
- Revise from leaves to root
- Root domain: values that belong to a solution



(Directional) AC solves Berge-acyclic CN

Tree CN

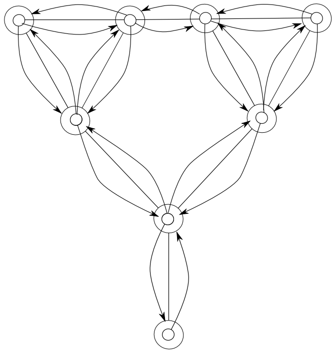
- Revise from leaves and back
- All domains: values that belong to a solution
- Resulting problem solved backtrack-free[19,18]



Can be done on any CN, with arbitrary graph

Arc consistency (Waltz 1972)

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



Thomas Schiex, Jean-Charles. Régin, Chistine Gaspin, and Gérard Verfaillie. "Lazy Arc Consistency". In: Proc. of AAAI'96. Portland, OR: AAAI Press, Aug. 1996

MP - Dynamic Programming[35,28]

1. Assume that the optimum cost on $x_1 \dots x_{i-1}$ is known for every value of D^{i-1}
2. We can extend this to D^i for $x_1 \dots x_i$
3. Let $f_i = \min_{x_{i-1}}(\varphi_{i-1} + \varphi_{i,i-1})$
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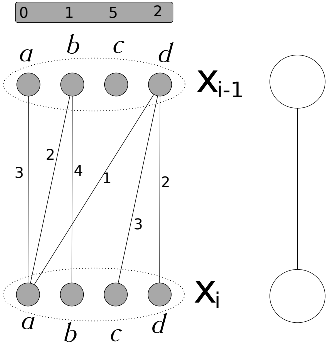

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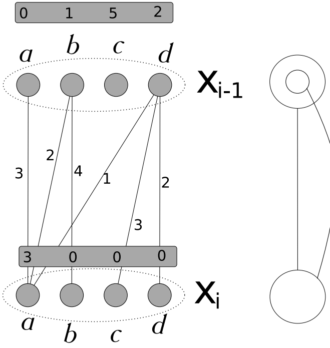

MRF/BN/Factor graphs (− log domain)

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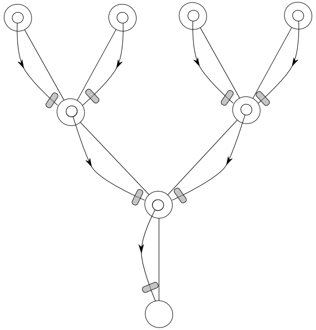

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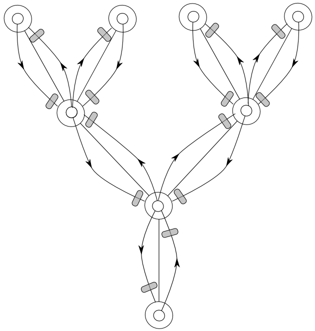

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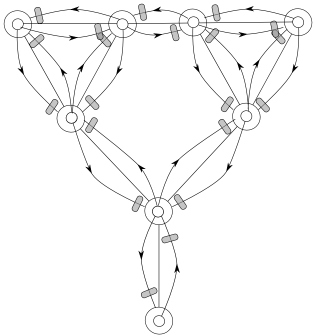

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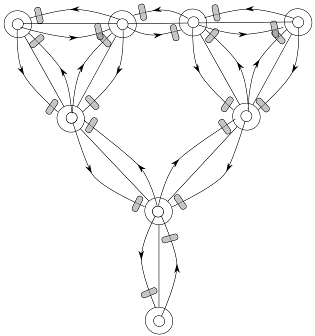
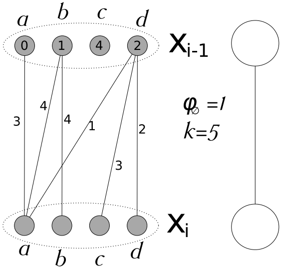


1. Solves Berge acyclic MRF/BN (acyclic Factor Graphs)
2. Does not converge on graphs (Loopy Belief Propagation)
3. Massively used to produce “good” solutions (turbo-decoding[39])
4. Not an equivalence preserving transformation!

Soft AC as Dynamic programming

1. use $\varphi_\varnothing$ and $\varphi_i(\cdot)$ to store optimum cost over $(x_1, \ldots, x_i)$
2. Preserves equivalence by "cost shifting"[45,53,42]



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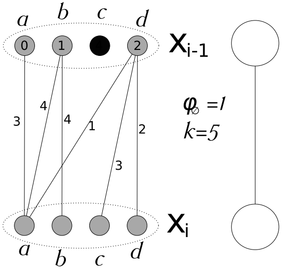

Soft Arc Consistency ≈ MP through transformation

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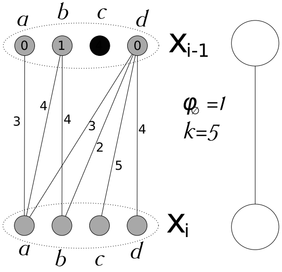

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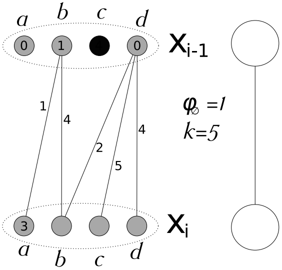

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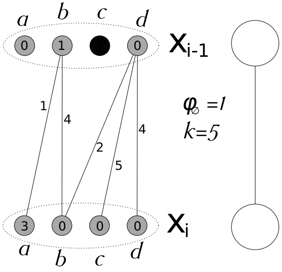
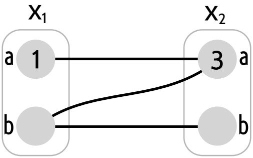


T. Schiex. "Arc consistency for soft constraints". In: Principles and Practice of Constraint Programming - CP 2000. Vol. 1894. LNCS. Singapore, Sept. 2000, pp. 411–424

Tightening by cost shifting

Assume that initially $\varphi_{\varnothing} = 0$, $k = 4$



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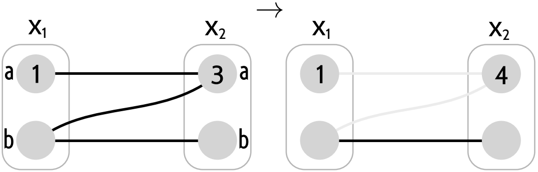
Assume that initially $\varphi_\varnothing = 0$, k $= 4$

Shift 1 to right a



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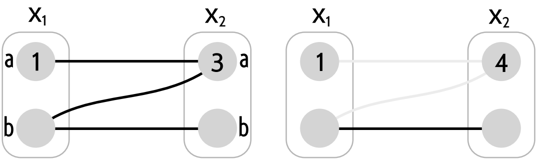

$\leftarrow$

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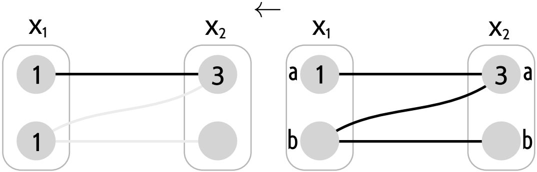
Assume that initially $\varphi_\varnothing = 0$, k $= 4$

Shift 1 to left b



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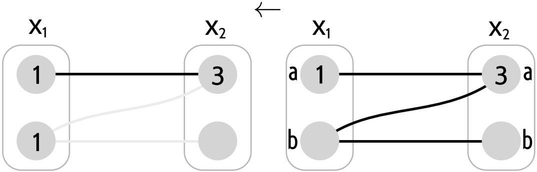

$\Downarrow$ Shift 1 from φ_1 to $\varphi_\varnothing$

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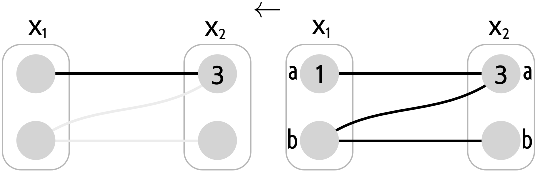

$\Downarrow$ Shift 1 from φ_1 to $\varphi_\varnothing$

$\varphi_\varnothing = 1$

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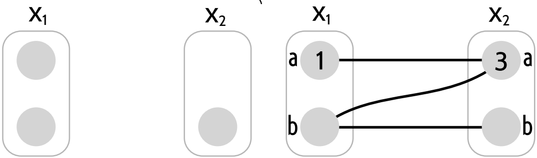

$\Downarrow$ Shift 1 from φ_1 to $\varphi_\varnothing$

$\varphi_\varnothing = 1$

Preserves the joint function F$(\cdot)$ below k

Properties

- Solves tree structured problems, optimum in $\varphi_\varnothing$
- Reformulation: incremental
- May loop indefinitely (graphs)
- No unique fixpoint (when it exists)
- Already used by Ukrainian school[45,27,26,54] and for a subclass of ILP.[53]
- Independently introduced in 2003 in ML as "reparametrizations"[51]

T. Schiex. "Arc consistency for soft constraints". In: Principles and Practice of Constraint Programming - CP 2000. Vol. 1894. LNCS. Singapore, Sept. 2000, pp. 411–424

M C. Cooper and T. Schiex. "Arc consistency for soft constraints". In: Artificial Intelligence 154.1-2 (2004), pp. 199–227

Convergent Soft Arc Consistencies

Breaking the loops, strengthening $\varphi_\varnothing$

1. 2000: Arc consistency[42,29]
2. 2003: Full Directional AC[6,31,32]
3. 2005: Existential DAC[30]
4. 2008: Virtual AC[10,9]
5. 2007: Optimal Soft AC[7] (LP)

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3. 2005: Existential DAC[30]
4. 2008: Virtual AC[10,9]
5. 2007: Optimal Soft AC[7] (LP)

- $O(ed)$ space, equivalent to the CSP variants on CSP (except OSAC).
- Implemented in **toulbar2**, with many other bells & whistles

Javier Larrosa and Thomas Schiex. "Solving weighted CSP by maintaining arc consistency". In: Artif. Intell. 159.1-2 (2004), pp. 1–26

M. Cooper, S. de Givry, M. Sanchez, T. Schiex, et al. "Soft arc consistency revisited". In: Artificial Intelligence 174 (2010), pp. 449–478

LP variables, binary CFN with no constraint/determinism

1. u_i: amount of cost shifted from φ_i to $\varphi_\varnothing$
2. q_{ija}: amount of cost shifted from φ_{ij} to $a \in D^i$

Optimal Soft Arc Consistency (finite costs, $k = \infty$)

LP variables, binary CFN with no constraint/determinism

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OSAC[45,25,7,54,9]

Maximize $\sum_{i=1}^{n} u_i$ subject to

$$\varphi_i(a) - u_i + \sum_{(\varphi_{ij} \in \Phi)} q_{ija} \geq 0 \qquad \forall i \in \{1, \dots, n\}, \forall a \in D^i$$

$$\varphi_{ij}(a, b) - q_{ija} - q_{jib} \geq 0 \qquad \forall \varphi_{ij} \in \Phi, \forall (a, b) \in D^{ij}$$

M C. Cooper, S. de Givry, and T. Schiex. "Optimal soft arc consistency". In: Proc. of IJCAI'2007. Hyderabad, India, Jan. 2007, pp. 68–73

Remember the local polytope ?

01 LP Variables, for a binary CFN

1. v_{ia}: value a used for variable x_i.
2. p_{iajb}: pair (a, b) used for x_i and x_j

The MRF local polytope[54]

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

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

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

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OSAC is its dual: u_i multiplier for (1) and q_{ija} for (2).

Better understanding

1. Soft convergent ACs find feasible (but non necessarily optimal) solutions of the dual.
2. Optimal does not mean more efficient for tree search.

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2015: universality of the local polytope

Prusa and Werner[38] showed that any "normal" LP can be reduced to such a polytope in linear time (constructive proof).

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2015: universality of the local polytope

Prusa and Werner[38] showed that any "normal" LP can be reduced to such a polytope in linear time (constructive proof).

Could soft arc consistency (eg. VAC) speed-up LP?

VAC faster than LP, close/same bound

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.
```

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CPLEX V12.4.0.0

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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.
```

Progress

Radio Link Frequency Assignment Problems

Assign frequencies to radio link in order to minimize interferences.

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
- More than 30,000 times faster
- All min-interference instances closed. Most resisted ILP (fap.zib.de)

B. Cabon, S. de Givry, L. Lobjois, T. Schiex, et al. "Radio Link Frequency Assignment". In: Constraints Journal 4 (1999), pp. 79–89

Computational Protein Design[48,1]

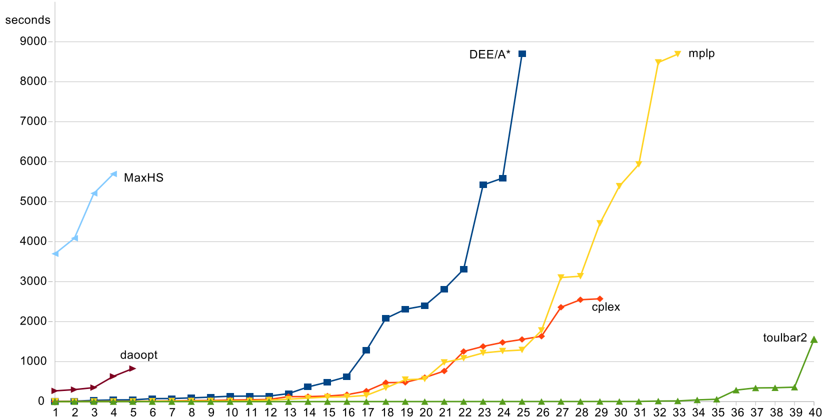
Design new enzymes for biofuels, drugs...cosmetics too

- graphical model capturing molecule stability based on atom-scale forces (electrostatics, solvation, torsion, Van der Waals...)

- Few variables (from 10 to few hundreds)
- Huge domains (typ. d $= 450$)
- Exact solvers: DEE/A* (DEE[14]), ILP[24]
- By far the most used: simulated annealing (Rosetta[21]).

Seydou Traoré, David Allouche, Isabelle André, Simon de Givry, et al. "A new framework for computational protein design through cost function network optimization". In: Bioinformatics 29.17 (2013), pp. 2129–2136

Multi-paradigm comparison - QP,SDP,ILP,Maxsat,MRF,CFN



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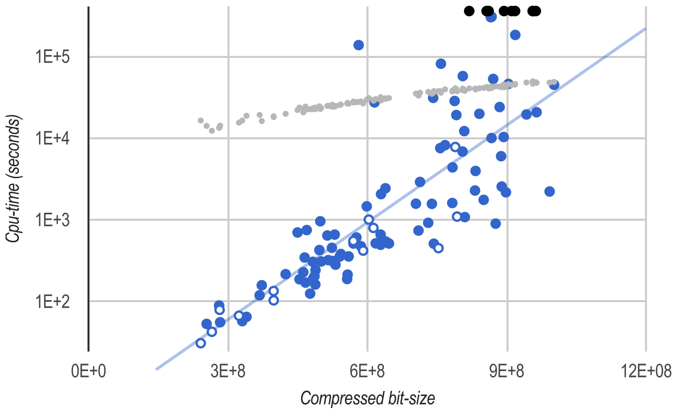
Faster than dedicated simulated annealing[46]



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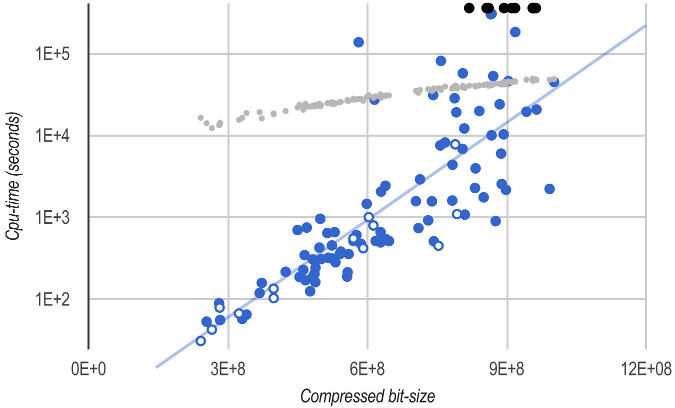

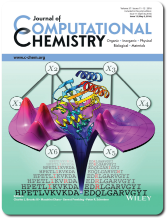

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Graphical models for biology

Genetic mapping with CarthaGene

GM learning + TSP optimization.

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RNA Gene finding: MilPat, Darn!

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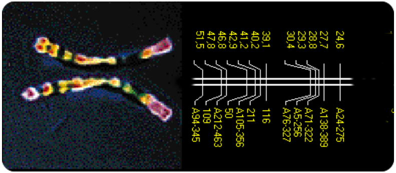

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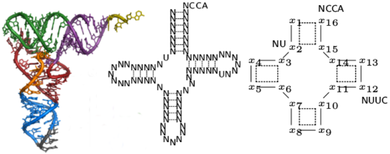

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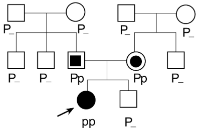

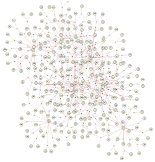

Beyond optimization

Graphical models with decision and stochastic variables

- MRF/BN: stochastic variables + probability distribution. Can be learnt (RBM for deep learning).
- CFN: decision variables + cost functions/utilities/feasibility distribution.

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Mixed graphical models with decision and stochastic variables

- Influence diagrams[22]
- Stochastic constraint programming[52]
- Plausability-feasibility-utility networks[37]

H. Fargier, J. Lang, R. Martin-Clouaire, and Thomas Schiex. "A constraint satisfaction framework for decision under uncertainty". In: Proc. of the 11th Int. Conf. on Uncertainty in Artificial Intelligence. Montréal, Canada, Aug. 1995

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C Pralet, G Verfaillie, and T Schiex. "An algebraic graphical model for decision with uncertainties, feasibilities, and utilities". In: Journal of Artificial Intelligence Research 29 (2007), pp. 421–489

Beyond NP

- Marginal probability: weighted counting[50]
- Marginal MAP: maximize probability with unobservable variables.
- Maximize expected utility...

Clément Viricel, David Simoncini, Sophie Barbe, and Thomas Schiex. "Guaranteed Weighted Counting for Affinity Computation: Beyond Determinism and Structure". In: International Conference on Principles and Practice of Constraint Programming. Springer. 2016, pp. 733–750

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Beyond optimization

Graphical models

Provide a strong and grounded basis for data analytics, from data to decision.

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Graphical models

Provide a strong and grounded basis for data analytics, from data to decision.

We need efficient anytime anyspace algorithms, with associated modelling langages and solvers.

Questions ?

References I

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