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

Thomas Schiex

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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

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.

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

Finding perfect solutions to perfectly defined problems

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The world is often more complex

ML gives us the capacity to build models of complex systems from data.

Early planning for GPS navigation

- A digital model of roads
- A shortest path algorithm for planning
- GPS navigation monitors plan execution

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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
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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 $X = \{x_1, \dots, x_n\}$ 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 , $\mathbf{x} \in D^X$:

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

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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).

Constraint Network

- 1 Variables and domains
- 2 φ_S are Boolean functions (constraints, $t \equiv 0 < 1 \equiv f$)
- 3 Minimize joint function ($\oplus = \wedge = \max$)

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

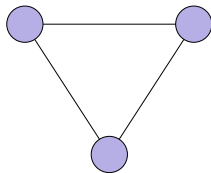
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Graph coloring/RLFAP-feas

- 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?



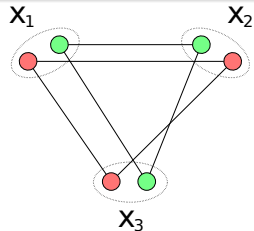
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Need to shift from perfect knowledge processing to approximate/imperfect knowledge processing

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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...)

T. Schiex, H. Fargier, and G. Verfaillie. "Valued Constraint Satisfaction Problems: hard and easy problems". In: Proc. of the 14th IJCAI. Montréal, Canada, Aug. 1995, pp. 631–637

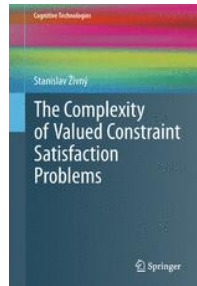
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Cost Function Networks - Weighted Constraint Networks - GAI models

- Variables and domains as usual
- Cost functions $\varphi_S : D^S \rightarrow \{0, \dots, k\}$ (k finite or not)
- Combined by bounded addition⁸

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

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 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:

$$p(X = \mathbf{x}) \propto \prod_{\varphi_S \in \Phi} \varphi_S(\mathbf{x}_S)$$

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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.

- 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

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

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

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

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

Continuous relaxation : the local polytope^{45,25,54}

Exact approaches (beyond ILP)

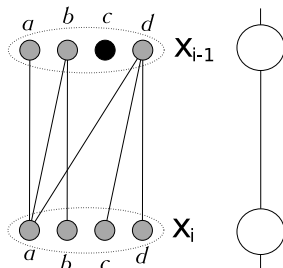
- 1 Dynamic programming (Variable and join-tree elimination,^{2,12} resolution^{11,40,13})
- 2 Tree search + fast, incremental approximate local reasoning (CP, SAT)

Fast, approximate reasoning with some guarantees

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

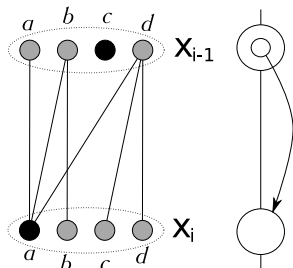
AC as Dynamic programming

- 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



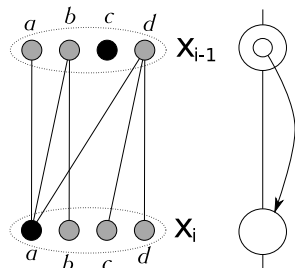
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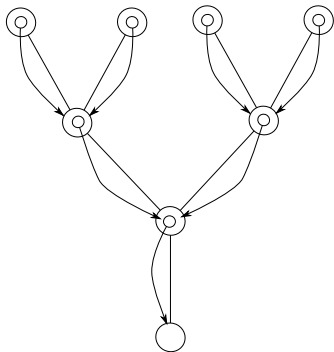


Revise: Equivalence Preserving Transformation

The resulting problem is equivalent (same set of solutions)

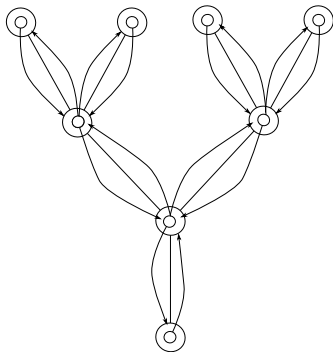
Rooted tree CN

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



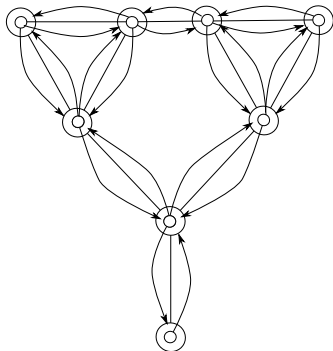
Tree CN

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



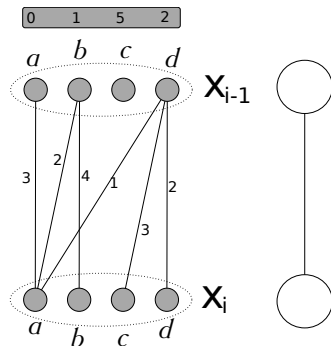
Arc consistency (Waltz 1972)

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



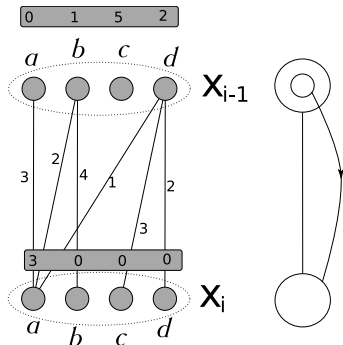
MP - Dynamic Programming^{35,28}

- 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 $f_i = \min_{x_{i-1}} (\varphi_{i-1} + \varphi_{i,i-1})$
- 4 Store f_i as a message



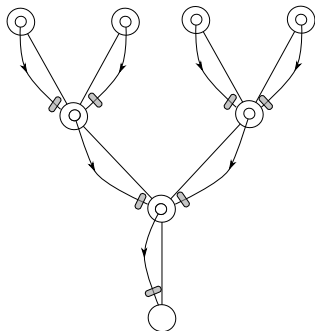
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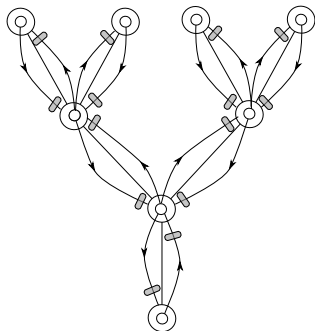
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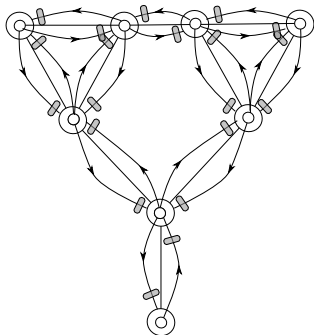
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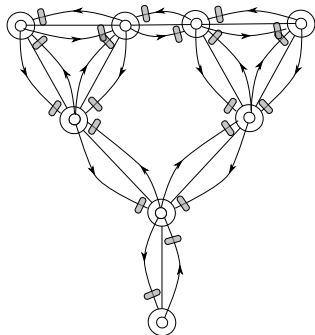
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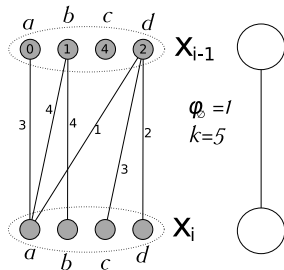
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- 1 Solves Berge acyclic MRF/BN (acyclic Factor Graphs)
- 2 Does not converge on graphs (Loopy Belief Propagation)
- 3 Massively used to produce “good” solutions (turbo-decoding³⁹)
- 4 Not an equivalence preserving transformation!

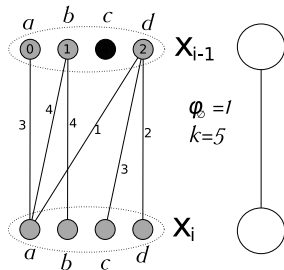
Soft AC as Dynamic programming

- 1 use φ_\emptyset and $\varphi_i(\cdot)$ to store optimum cost over (x_1, \dots, x_i)
- 2 Preserves equivalence by “cost shifting”^{45,53,42}



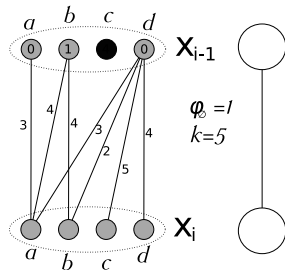
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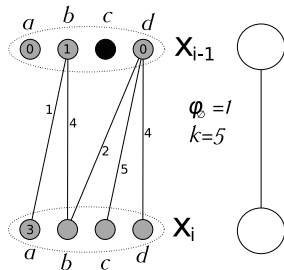
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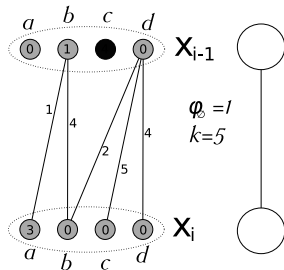
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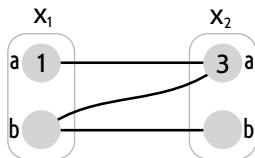


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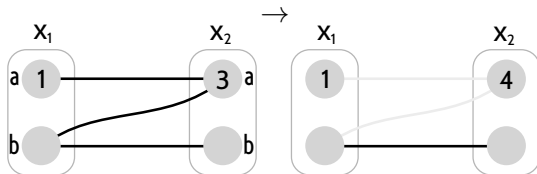


Assume that initially $\varphi_{\emptyset} = 0, k = 4$

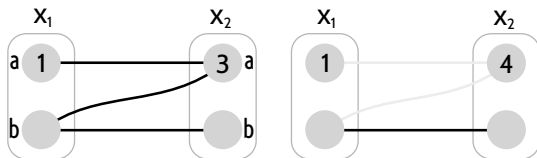


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Shift 1 to right a



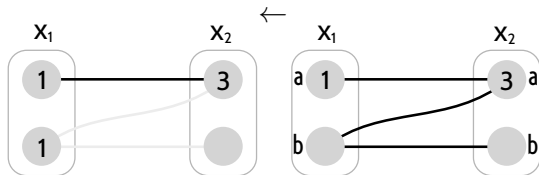
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Shift 1 from right a

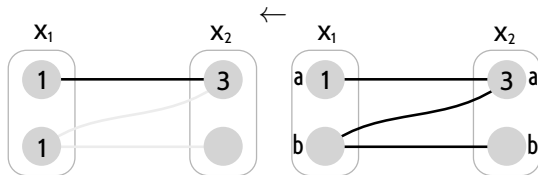
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Shift 1 to left b



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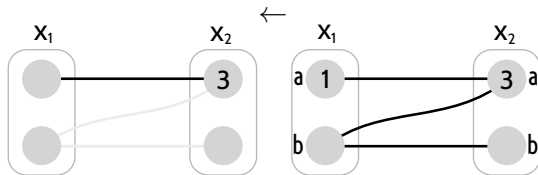
Shift 1 to left b



⇓ Shift 1 from φ_1 to φ_{\emptyset}

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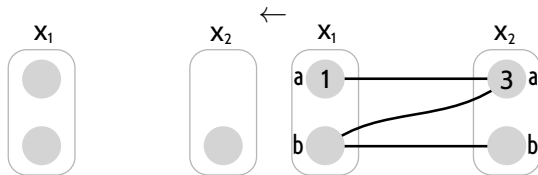


⇓ Shift 1 from φ_1 to φ_{\emptyset}

$$\varphi_{\emptyset} = 1$$

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

Shift 1 to left b



⇓ Shift 1 from φ_1 to φ_\emptyset

$$\varphi_\emptyset = 1$$

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

- Solves tree structured problems, optimum in φ_0
- 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

Breaking the loops, strengthening φ_0

- 1 2000: Arc consistency^{42,29}
- 2 2003: Full Directional AC^{6,31,32}
- 3 2005: Existential DAC³⁰
- 4 2008: Virtual AC^{10,9}
- 5 2007: Optimal Soft AC⁷ (LP)

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- 0(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_j : amount of cost shifted from φ_i to φ_\emptyset
- 2 q_{ija} : amount of cost shifted from φ_{ij} to $a \in D^i$

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OSAC^{45,25,7,54,9}

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

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 polytope⁵⁴

$$\begin{aligned} \text{Minimize } & \sum_{i,a} c_i(a) \cdot x_{ia} + \sum_{\substack{c_{ij} \in C \\ a \in D^i, b \in D^j}} c_{ij}(a, b) \cdot y_{iajb} \quad \text{s.t} \\ & \sum_{a \in D^i} x_{ia} = 1 & \forall i \in \{1, \dots, n\} & \quad (1) \\ & \sum_{b \in D^j} y_{iajb} - x_{ia} = 0 & \forall c_{ij}/c_{ji} \in C, \forall a \in D^i & \quad (2) \end{aligned}$$

Remember the local polytope ?

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- 2 p_{iajb} : pair (a, b) used for x_i and x_j

The MRF local polytope⁵⁴

$$\begin{aligned} \text{Minimize } & \sum_{i,a} c_i(a) \cdot x_{ia} + \sum_{\substack{c_{ij} \in C \\ a \in D^i, b \in D^j}} c_{ij}(a, b) \cdot y_{iajb} \text{ s.t} \\ & \sum_{a \in D^i} x_{ia} = 1 & \forall i \in \{1, \dots, n\} & \quad (1) \\ & \sum_{b \in D^j} y_{iajb} - x_{ia} = 0 & \forall c_{ij}/c_{ji} \in C, \forall a \in D^i & \quad (2) \end{aligned}$$

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

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- 2 Optimal does not mean more efficient for tree search.

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2015: universality of the local polytope

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

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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```

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.
```

Radio Link Frequency Assignment Problems

Assign frequencies to radio link in order to minimize interferences.

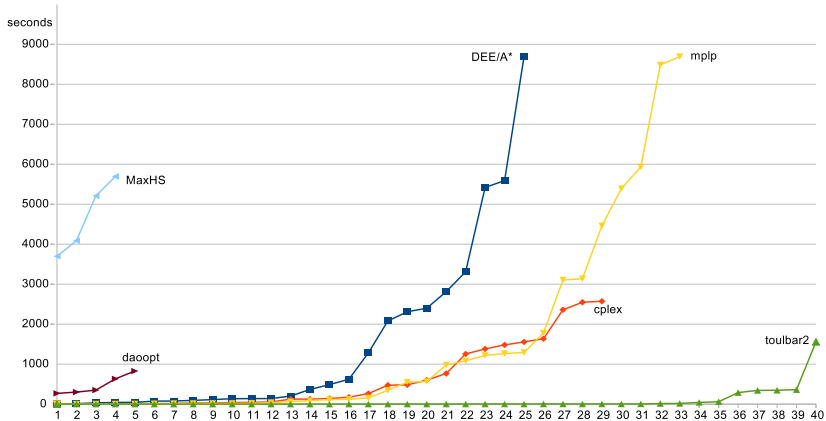
CELAR 06, $n = 100$, $d = 44$ - one core

- 1 1997: 26 days on 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)

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* (DEE¹⁴), ILP²⁴
- By far the most used: simulated annealing (Rosetta²¹).

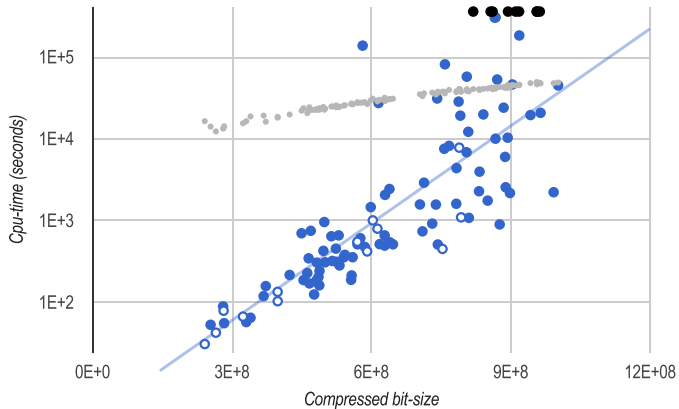
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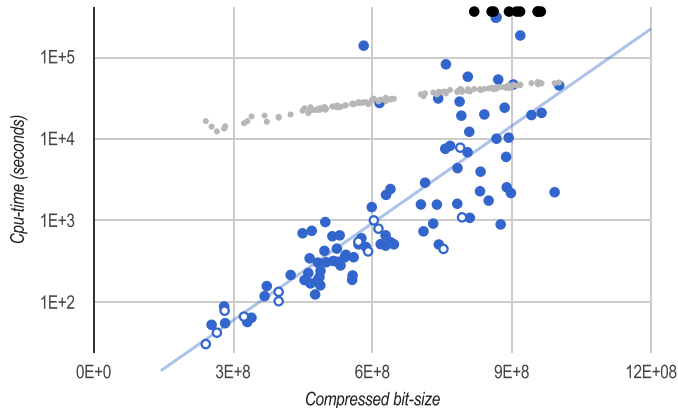
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Faster than dedicated simulated annealing⁴⁶



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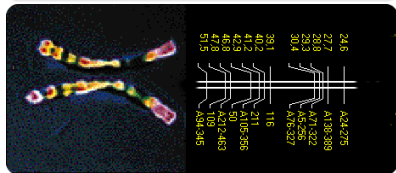
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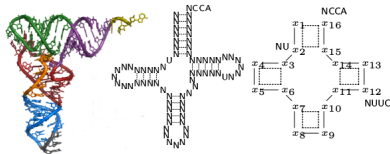
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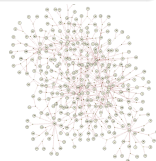
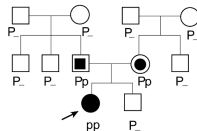
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Graphical models with decision and stochastic variables

- MRF/BN: stochastic variables + probability distribution. Can be learnt (RBM for deep learning).
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Mixed graphical models with decision and stochastic variables

- Influence diagrams²²
- Stochastic constraint programming⁵²
- Plausability-feasibility-utility networks³⁷

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

H. Fargier, J. Lang, and T. Schiex. "Mixed Constraint Satisfaction: a framework for decision problems under incomplete knowledge". In: Proc. of AAAI'96. Portland, OR: AAAI Press, Aug. 1996

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 counting⁵⁰
- 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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Graphical models

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

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

Questions ?

- [1] David Allouche, Isabelle André, Sophie Barbe, Jessica Davies, et al. “Computational protein design as an optimization problem”. In: *Artificial Intelligence* 212 (2014), pp. 59–79.
- [2] Umberto Bertelé and Francesco Briosi. *Nonserial Dynamic Programming*. Academic Press, 1972.
- [3] S. Bistarelli, H. Fargier, U. Montanari, F. Rossi, et al. “Semiring-based CSPs and Valued CSPs: Frameworks, Properties and Comparison”. In: *Constraints* 4 (1999), pp. 199–240.
- [4] B. Cabon, S. de Givry, L. Lobjois, T. Schiex, et al. “Radio Link Frequency Assignment”. In: *Constraints Journal* 4 (1999), pp. 79–89.
- [5] Tomato Genome Consortium et al. “The tomato genome sequence provides insights into fleshy fruit evolution”. In: *Nature* 485.7400 (2012), pp. 635–641.
- [6] M C. Cooper. “Reduction operations in fuzzy or valued constraint satisfaction”. In: *Fuzzy Sets and Systems* 134.3 (2003), pp. 311–342.
- [7] 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.
- [8] M C. Cooper and T. Schiex. “Arc consistency for soft constraints”. In: *Artificial Intelligence* 154.1-2 (2004), pp. 199–227.
- [9] M. Cooper, S. de Givry, M. Sanchez, T. Schiex, et al. “Soft arc consistency revisited”. In: *Artificial Intelligence* 174 (2010), pp. 449–478.

- [10] Martin C Cooper, Simon de Givry, Martí Sánchez, Thomas Schiex, et al. "Virtual Arc Consistency for Weighted CSP." In: AAAI. Vol. 8. 2008, pp. 253–258.
- [11] Martin Davis and Hilary Putnam. "A computing procedure for quantification theory". In: Journal of the ACM (JACM) 7.3 (1960), pp. 201–215.
- [12] Rina Dechter. "Bucket Elimination: A Unifying Framework for Reasoning". In: Artificial Intelligence 113.1–2 (1999), pp. 41–85.
- [13] Rina Dechter and Irina Rish. "Directional resolution: The Davis–Putnam procedure, revisited". In: KR 94 (1994), pp. 134–145.
- [14] J Desmet, M De Maeyer, B Hazes, and I Lasters. "The dead-end elimination theorem and its use in protein side-chain positioning." In: Nature 356.6369 (Apr. 1992), pp. 539–42. ISSN: 0028-0836.
- [15] T. Faraut, S. de Givry, P. Chabrier, T. Derrien, et al. "A comparative genome approach to marker ordering." In: Bioinformatics 23.2 (2007), e50–6.
- [16] 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.
- [17] H. Fargier, J. Lang, and T. Schiex. "Mixed Constraint Satisfaction: a framework for decision problems under incomplete knowledge". In: Proc. of AAAI'96. Portland, OR: AAAI Press, Aug. 1996.

- [18] Eugene C. Freuder. "A sufficient Condition for Backtrack-Bounded Search". In: *Journal of the ACM* 32.14 (1985), pp. 755–761.
- [19] Eugene C. Freuder. "A sufficient Condition for Backtrack-free Search". In: *Journal of the ACM* 29.1 (1982), pp. 24–32.
- [20] S. de Givry, M. Bouchez, P. Chabrier, D. Milan, et al. "CarthaGene: multipopulation integrated genetic and radiation hybrid mapping." In: *Bioinformatics* 21.8 (2005), pp. 1703–4.
- [21] Dominik Gront, Daniel W Kulp, Robert M Vernon, Charlie EM Strauss, et al. "Generalized fragment picking in Rosetta: design, protocols and applications". In: *PLoS one* 6.8 (2011), e23294.
- [22] Ronald A Howard and James E Matheson. "Influence diagrams". In: *Decision Analysis* 2.3 (2005), pp. 127–143.
- [23] Barry Hurley, Barry O'Sullivan, David Allouche, George Katsirelos, et al. "Multi-language evaluation of exact solvers in graphical model discrete optimization". In: *Constraints* 21.3 (2016), pp. 413–434.
- [24] Carleton L Kingsford, Bernard Chazelle, and Mona Singh. "Solving and analyzing side-chain positioning problems using linear and integer programming." In: *Bioinformatics (Oxford, England)* 21.7 (Apr. 2005), pp. 1028–36. ISSN: 1367-4803.
- [25] A M C A. Koster. "Frequency assignment: Models and Algorithms". Available at www.zib.de/koster/thesis.html. PhD thesis. The Netherlands: University of Maastricht, Nov. 1999.

- [26] VK Koval' and Mykhailo Ivanovich Schlesinger. "Two-dimensional programming in image analysis problems". In: *Avtomatika i Telemekhanika* 8 (1976), pp. 149–168.
- [27] VA Kovalevsky and VK Koval. "A diffusion algorithm for decreasing energy of max-sum labeling problem". In: *Glushkov Institute of Cybernetics, Kiev, USSR* (1975).
- [28] Frank R Kschischang, Brendan J Frey, and Hans-Andrea Loeliger. "Factor graphs and the sum-product algorithm". In: *Information Theory, IEEE Transactions on* 47.2 (2001), pp. 498–519.
- [29] J. Larrosa. "On Arc and Node Consistency in weighted CSP". In: *Proc. AAAI'02, Edmondton, (CA), 2002*, pp. 48–53.
- [30] J. Larrosa, S. de Givry, F. Heras, and M. Zytnicki. "Existential arc consistency: getting closer to full arc consistency in weighted CSPs". In: *Proc. of the 19th IJCAI, Edinburgh, Scotland, Aug. 2005*, pp. 84–89.
- [31] J. Larrosa and T. Schiex. "In the quest of the best form of local consistency for Weighted CSP". In: *Proc. of the 18th IJCAI, Acapulco, Mexico, Aug. 2003*, pp. 239–244.
- [32] Javier Larrosa and Thomas Schiex. "Solving weighted CSP by maintaining arc consistency". In: *Artif. Intell.* 159.1–2 (2004), pp. 1–26.
- [33] V. Laurent, E. Wajnberg, B. Mangin, T. Schiex, et al. "A composite genetic map of the parasitoid wasp *Trichogramma brassicae* based on RAPD markers." In: *Genetics* 150.1 (1998), pp. 275–82.
- [34] C. Mathé, M. F. Sagot, T. Schiex, and P. Rouzé. "Current methods of gene prediction, their strengths and weaknesses." In: *Nucleic Acids Res* 30.19 (2002), pp. 4103–17.

- [35] Judea Pearl. Probabilistic Reasoning in Intelligent Systems, Networks of Plausible Inference. Palo Alto: Morgan Kaufmann, 1988.
- [36] C Pralet, T Schiex, and G Verfaillie. "From influence diagrams to multioperator cluster DAGs". In: Proc. of UAI'2006. Boston, MA, 2006.
- [37] 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.
- [38] Daniel Prusa and Tomas Werner. "Universality of the local marginal polytope". In: Pattern Analysis and Machine Intelligence, IEEE Transactions on 37.4 (2015), pp. 898-904.
- [39] Thomas J Richardson and Rüdiger L Urbanke. "The capacity of low-density parity-check codes under message-passing decoding". In: Information Theory, IEEE Transactions on 47.2 (2001), pp. 599-618.
- [40] J. Alan Robinson. "A machine-oriented logic based on the resolution principle". In: Journal of the ACM 12 (1965), pp. 23-44.
- [41] M Sanchez, S de Givry, and T Schiex. "Mendelian error detection in complex pedigrees using weighted constraint satisfaction techniques". In: Constraints 13.1 (2008), pp. 130-154.
- [42] 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.
- [43] T. Schiex, H. Fargier, and G. Verfaillie. "Valued Constraint Satisfaction Problems: hard and easy problems". In: Proc. of the 14th IJCAI. Montréal, Canada, Aug. 1995, pp. 631-637.

- [44] Thomas Schiex, Jean-Charles Régim, Christine Gaspin, and Gérard Verfaillie. “Lazy Arc Consistency”. In: Proc. of AAAI’96. Portland, OR: AAAI Press, Aug. 1996.
- [45] M.I. Schlesinger. “Sintaksicheskiy analiz dvumernykh zritelnykh signalov v usloviyakh pomekh (Syntactic analysis of two-dimensional visual signals in noisy conditions)”. In: Kibernetika 4 (1976), pp. 113–130.
- [46] David Simoncini, David Allouche, Simon de Givry, Celine Delmas, et al. “Guaranteed discrete energy optimization on large protein design problems”. In: Journal of chemical theory and computation 11.12 (2015), pp. 5980–5989.
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- [51] Martin J Wainwright, Tommi S Jaakkola, and Alan S Willsky. "Tree-based reparameterization framework for analysis of sum-product and related algorithms". In: *IEEE Transactions on information theory* 49.5 (2003), pp. 1120–1146.
- [52] Toby Walsh. "Stochastic constraint programming". In: *ECAI*. Vol. 2. 2002, pp. 111–115.
- [53] Dag Wedelin. "An algorithm for large scale 0–1 integer programming with application to airline crew scheduling". In: *Annals of operations research* 57.1 (1995), pp. 283–301.
- [54] T. Werner. "A Linear Programming Approach to Max-sum Problem: A Review." In: *IEEE Trans. on Pattern Recognition and Machine Intelligence* 29.7 (July 2007), pp. 1165–1179. URL: <http://dx.doi.org/10.1109/TPAMI.2007.1036>.
- [55] M Zytynicki, C Gaspin, and T Schiex. "DARN! A soft constraint solver for RNA motif localization". In: *Constraints* 13.1 (2008), pp. 91–109.