

Optimization in Graphical Models

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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)

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

Powering computer (and other) science areas

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

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



Informal

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



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Why Graphical ?

- a vertex per variable, a (hyper)edge per function
- Or its incidence graph (Factor graphs²⁸)
- Illows to describe knowledge on a lot of variables concisely
- Usually hard to manipulate (NP-hard queries).

A Constraint Network is a GM



Constraint Network

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

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

A Constraint Network is a GM

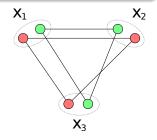
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Graph coloring/RLFAP-feas

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







SAT

- Variables x_i are boolean ($0 \equiv true, 1 \equiv false$)
- Constraints are defined as clauses $I_{i_1} \vee \cdots \vee I_{i_p}$ I_i is x_i or $\bar{x}_i = (1 - x_i)$ (negation).
- $\textbf{S} \text{ Truth value: } (I_{i_1} \vee \cdots \vee I_{i_p}) = I_{i_1} \times \cdots \times I_{i_p}$

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



Simply

Shift from boolean functions to cost functions

Lifting CSP to optimization



Cost Function Networks - Weighted Constraint Networks

- Variables and domains as usual
- Cost functions $W \ni c_S : D^S \to \{0, \ldots, k\}$ (k finite or not)
- Cost combined by (bounded) addition⁸ (other, see VCSP⁴⁶).

$$cost(t) = \sum_{c_{\mathcal{S}} \in C} c_{\mathcal{S}}(t[\mathcal{S}]) \qquad c_{\varnothing} : ext{lower bound}$$

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



Cost Function Networks - Weighted Constraint Networks

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

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

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: $(I_{i_1} \lor \cdots \lor I_{i_p}, v_i) = v_i \times (I_{i_1} \times \cdots \times I_{i_p})$
- Minimize the sum of all these.
- Polynomial Pseudo-Boolean Optimization.⁵
- 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:

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

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. Binary MRF/CFN as 01LP (infinite k, finite costs)



01 LP Variables, for a binary MRF/CFN

•
$$x_{ia}$$
: value a used for variable x_i .

3
$$y_{iajb}$$
: pair (a, b) used for x_i and x_j

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

$$\begin{array}{ll} \sum_{a \in D^i} x_{ia} = 1 & \forall i \in \{1,\ldots,n\} \\ \sum_{b \in D^j} y_{iajb} = x_{ia} & \forall c_{ij} \in C, \forall a \in D^i \\ x_{ia}, y_{iajb} \in \{0,1\} \end{array}$$

Linear relaxation : the local polytope^{47,25,53}

Exact approaches (beyond ILP)

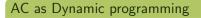
- Full dynamic programming (Variable elimination,^{3,13} resolution^{12,43,14})
- Tree search + fast, incremental approximate local reasoning

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

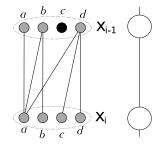
Arc Consistency = local dynamic programming





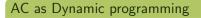
- Imagine a CSP with linear graph
- Which values of x_i belong to a solution of x₁,...x_i knowing those for x_{i-1}.

•
$$\min_{x_{i-1}}(\max(c_{i-1}, c_{i,i-1}))$$



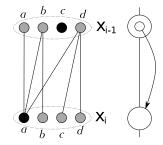
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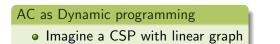
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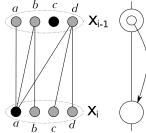
Arc Consistency = local dynamic programming





Which values of x_i belong to a solution of x₁,...x_i knowing those for x_{i-1}.

•
$$\min_{x_{i-1}}(\max(c_{i-1}, c_{i,i-1}))$$



Revise = Equivalence Preserving Transformation (EPT)

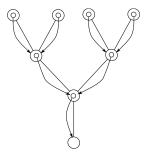
- $\nexists b \in D^j \mid c_{ij}(a, b) = 0.$
- we can delete a in c_i (or D^i).
- the resulting problem is equivalent (same set of solutions)

(Directional) AC solves Berge-acyclic CN



Rooted tree CN

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

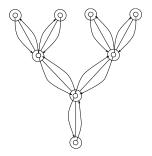


(Directional) AC solves Berge-acyclic CN



Tree CN

- Revise from leaves and back
- All domains: values that belong to a solution
- Resulting problem solved backtrack-free^{20,19}



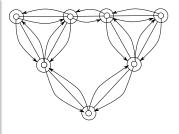
Can be done on any CN, with arbitrary graph



Arc consistency (Waltz 72)

- Linear time (tables)
- Oligie Unique fixpoint (confluent)
- In Preserves equivalence
- May detect infeasibility
- Problem transformation (incremental)

Maintaining AC during search.



Unit Propagation as Dynamic programming



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

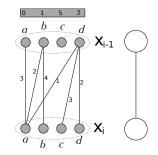
Maintaining UP during search (DPLL, ancestor of CDCL)



MP - Dynamic Programming^{40,28}

 optimum cost from x₁ to a ∈ D_i knowing those for x_{i-1}

2
$$\min_{x_{i-1}}(c_{i-1}+c_{i,i-1})$$

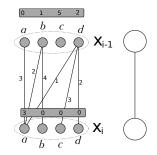




MP - Dynamic Programming^{40,28}

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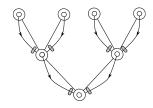




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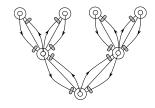




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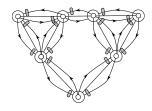




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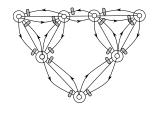
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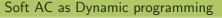
MP - Dynamic Programming^{40,28}

- Optimum cost from x₁ to a ∈ D_i knowing those for x_{i−1}
- $\bigcirc \min_{x_{i-1}}(c_{i-1}+c_{i,i-1})$
- Use external functions (messages) to store DP results

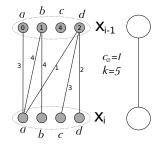


- Solves Berge acyclic MRF/BN (acyclic Factor Graphs)
- Ooes not converge on graphs (Loopy Belief Propagation)
- Massively used to produce "good" solutions (turbo-decoding⁴²)
- More recently introduced in Distributed COP¹⁸
- In Not an equivalence preserving transformation⁴⁰

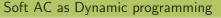




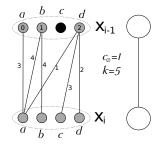
- MRF message passing but...
- ② use c_∅ and c_i(·) to store optimum cost from x₁ to x_i
- Preserves equivalence by "cost shifting" ^{47,52,45}



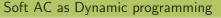




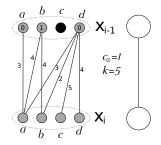
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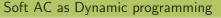




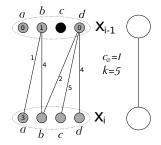
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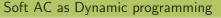




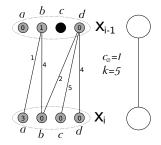
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Equivalence Preserving Transformation



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

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

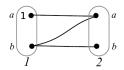
```
Precondition: -c_i(a) \le \alpha \le \min_{t' \in D^{ij}, t'[i]=a} c_{ij}(t');

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

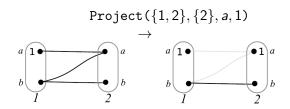
\begin{vmatrix} c_i(a) \leftarrow c_i(a) + \alpha; \\ \text{foreach } (t' \in D^{ij} \text{ such that } t'[i] = a, c_{ij}(t') < k) \text{ do} \\ | c_{ij}(t') \leftarrow c_{ij}(t') - \alpha; \\ \text{end} \end{vmatrix}
```

Example

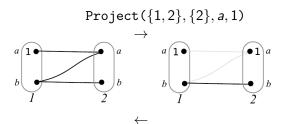






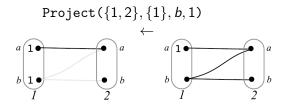




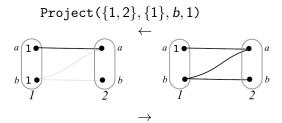


 $Project(\{1,2\},\{2\},a,-1)$



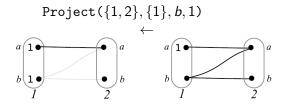






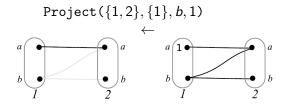
 $\texttt{Project}(\{1,2\},\{1\},b,-1)$





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





 \Downarrow Project ({1}, arnothing, [], 1) $c_{arnothing} = 1$



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

Convergent Soft Arc Consistencies

Breaking the loops

- Arc consistency: prevent loops at the arc level⁴⁵
- O Node consistency³⁰
- Oirectional AC: prevent loops at a global level^{6,32,33}
- Combine AC and DAC into FDAC^{32,33}
- **(**) Pool costs from all stars to c_{\emptyset} in EAC³⁴
- O Combine AC+DAC+EAC in EDAC³⁴

All O(ed) space. Equivalent to their "CSP" counterpart on constraints.

Max SAT Unit propagation (resolution)



Semantically, it's the the same

- Problems with leftovers after cost shifting
- Includes non CNF (Heras, Larrosa³¹)
- Represented as a linear number of "compensation clauses"⁴



Finding an optimal order⁸

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



Finding an optimal order⁸

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

Finding an optimal set⁷

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

LP Variables, for a binary CFN

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

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

LP Variables, for a binary CFN

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

OSAC

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

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

OSAC is the dual of the local polytope



01 LP Variables, for a binary CFN

1
$$x_{ia}$$
: value *a* used for variable x_i .

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

The MRF local polytope⁵³

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

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



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



2015

Prusa and Werner⁴¹ 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?

Can we organize our EPTs better w/o LP?



$Bool(P)^{10}$

Given a CFN P = (X, D, C, k)Bool(P) is the CSP $(X, D, C - \{c_{\varnothing}\}, 1)$.

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

Can we organize our EPTs better w/o LP?



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Virtual AC

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

Can we organize our EPTs better w/o LP?



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Virtual AC and MP

TRW-S,²⁴ MPLP1,⁴⁹ SRMP,²³ Max-Sum diffusion,^{27,11} Aug-DAG²⁶ converge to fixpoints that satisfy the same property.



Solutions of Bool(P) are optimal in P.



Solutions of Bool(P) are optimal in P.

VAC

- solves tree-structured problems,
- Solves CFNs with submodular cost functions (Monge matrices)
- Solves CFNs for which AC is a decision procedure in Bool(P).
- If P is VAC and one value a in each domain such that c_i(a) = 0 is solved.
- So 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). Progress: Radio Link Frequency Assignment (tb2)

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

- 1997: 26 days of a Sun UltraSparc 167 MHz.
- 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)

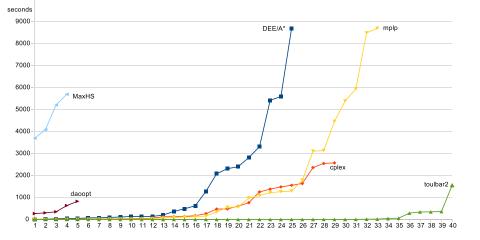


Design new enzymes for biofuels, drugs...cosmetics too

- 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 (DEE¹⁵), ILP²²
- By far most used: simulated annealing (Rosetta²¹).

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





Here, VAC faster than LP, often close/same bound



CPLEX V12.4.0.0

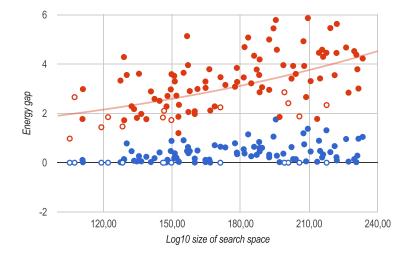
```
Problem '3e4h.LP' read.
Root relaxation solution time = 811.28 sec.
...
MIP - Integer optimal solution: Objective = 150023297067
Solution time = 864.39 sec.
```

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.

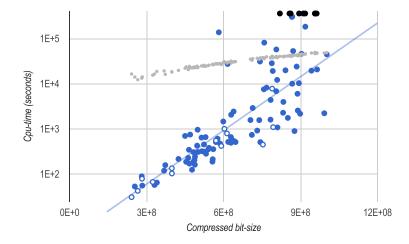
Exact (simulated annealing is stochastic)⁴⁸





Faster than dedicated simulated annealing⁴⁸





mulcyber.toulouse.inra.fr/projects/toulbar2



- First/second in approximate graphical model MRF/MAP challenges (2010, 2012, 2014).
- Global cost functions (weighted Regular, AllDiff, GCC...)
- Bioinformatics: pedigree debugging,⁴⁴ Haplotyping (QTLMap), structured RNA gene finding⁵⁴
- Inductive Logic Programming,² Natural Langage Processing (in hltdi-l3), Multi-agent and cost-based planning,^{29,9} Model Abstraction,⁵⁰ diagnostic,³⁶ Music processing and Markov Logic,^{39,38} Data mining,³⁷ Partially observable Markov Decision Processes,¹⁶ Probabilistic counting¹⁷ and inference,³⁵...



Everything is connected :-) Questions ?

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