## Numbers and logic together in CP:

 A Practical View of Cost Function NetworksS. de Givry ${ }^{1}$ \& T. Schiex ${ }^{1}$
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This is not a virtual tutorial
September 2020

Informally
A description of a multivariate function as the combination of a set of simple functions

## Concisely describing and analyzing complex systems

- Concise: we use a set of small functions
- Complex: the joint function results from the interaction of several small functions

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- A 3D molecule [All+14]

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- A pedigree with genotypes [SGS08]
- A frequency assignment [Cab+99]
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## Notations

- Variables: $X, Y, Z, \ldots$, possibly indexed as $X_{i}$
- Domains: $D^{X}$ for variable $X$, or $D^{i}$ for variable $X_{i}$
- Unknown values: $u, v, w, x, y, z \ldots$
- Sequence of variables: $X, Y, Z \ldots$
$\square$ Sequence of possible values: $u, v, w, x, y, z \ldots$
- Domain of a sequence of variables $X: D^{X}$ (Cartesian product of the domains)
- $u \in D^{X}$ is an assignment of $\boldsymbol{X}$ (a value for each variable in $\boldsymbol{X}$ )
- $u[Y]$ : projection of $u$ on $Y$ (the sequence of values of $Y$ in $u$ )


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Definition (Graphical Model (GM [Biso6; KFo9]))
A $\mathrm{GM} \mathcal{M}=\langle V, \Phi\rangle$ is defined by:

- a sequence of variables $V$
- each $X \in V$ has finite domain $D^{X}$
- a set $\Phi$ of functions (or factors)
- Each function $\varphi_{S} \in \Phi$ is a function from $D^{S} \rightarrow B$


## Definition ( $\mathcal{M}$ joint function)

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\Phi_{\mathcal{M}}(v)=\bigoplus_{\varphi_{S} \in \Phi} \varphi_{S}(v[S])
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- Default: as tensors over $B$
(multidimensional tables) (disjunction of variables or their negation)
- Arithmetic, polynomes [BH02]
- Predicates (All-Different [Rég94 LLL12]....)

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Constraint networks [RBWOG]/SAT [BHMO9]

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\Phi_{\mathcal{M}}=\bigwedge_{\varphi_{S} \in \Phi} \varphi_{S}
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## Markov Random Fields: $B=\mathbb{R}^{+}, \oplus=\times$

- a set $V$ of domain variables
- a set $\Phi$ of potential functions
- $\varphi_{S} \in \Phi: \prod_{X \in S} D^{X} \rightarrow \mathbb{R}^{+}$


## $\mathcal{M}$ : induces a probability distribution

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## Cost Function Networks $\mathcal{M}$ [FW92; SFV95; CS04] <br> $$
B=\overline{\mathbb{N}}^{k}, \oplus=\downarrow^{k}
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- a sequence of domain variables $V$
- a set $\Phi$ of $e$ numerical functions
- Each function $\varphi_{S} \in \Phi$ is a function from $D^{S} \rightarrow \overline{\mathbb{N}}^{k}$

■ $\overline{\mathbb{N}}^{k}$ : elements of $\mathbb{N} \cup\{\infty\}$ bounded by $k$
$k$ finite or not
$\square{ }^{k}$ is the $k$-bounded addition $\alpha+^{k} \beta=\min (\alpha+\beta, k)$

## $\mathcal{M}$ defines a joint (bounded) integer function



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\Phi_{\mathcal{M}}=\sum_{\varphi_{S} \in \Phi}^{k} \varphi_{S}
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- Have a constant function $\varphi \varnothing$
- Have all their unary functions $\varphi_{i}, X_{i} \in V \quad \varphi_{i}(u)=k$ means $u$ deleted
- All functions have different scopes


## Main properties

$\square \varphi_{\varnothing}$ is a lower bound of the joint function $\Phi_{\mathcal{M}}$
$\square k=1$ : Constraint networks and SAT, $+^{k}$ is $\wedge$

Graph $G=(\boldsymbol{V}, \boldsymbol{E})$ with edge weight function $w$

- A Boolean variable $X_{i}$ per vertex $i \in V$
- A cost function per edge $e=(i, j) \in E: \varphi_{i j}=w(i, j) \times \mathbb{1}\left[x_{i} \neq x_{j}\right]$
- Hard edges: constraints with costs 0 or $\infty\left(\right.$ when $\left.x_{i} \neq x_{j}\right)$


## A simple graph

- vertices $\{1,2,3,4\}$
- cut weight 1
- edge $(1,2)$ hard


## Example: Min-CUT with hard edges

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Min-CUT on 4 variables with hard edge
\{
problem :\{name: "MinCut", mustbe: "<100.0"\}, variables: \{x1: ["1"], x2: ["1","r"], x3: ["1","r"], x4: ["r"]\} functions: \{ cut12: \{scope: ["x1","x2"], costs: [0.0, 100.0, 100.0, 0.0]\}, cut13: \{scope: ["x1","x3"], costs: [0.0,1.0,1.0,0.0]\}, cut23: \{scope: ["x2","x3"], costs: [0.0,1.0,1.0,0.0]\}, cut34: \{scope: ["x3", "x4"], costs: [0.0,1.0,1.0,0.0]\}
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Definition (Functions and graphical models equivalence)
Two functions (or GMs) are equivalent iff they are always equal

Definition (Relaxation of a function or graphical model)
A function (or GM) $\varphi$ is a relaxation of $\varphi^{\prime}$ iff $\varphi \leq \varphi^{\prime}$
For $B=\mathbb{B}, t<f$

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2 Algorithms

3 All Toulbar2 bells and whistles

4 Learning CFN from data

Minimization queries

- $B=\{t \equiv 0, f \equiv 1\}, \oplus=廿^{1}=\wedge$, clauses
the SAT Problem
■ $B=\{t \equiv 0, f \equiv 1\}, \oplus=+\frac{1}{+}=\wedge$, tensors
the Constraint Satisfaction Problem
- $B=\overline{\mathbb{N}}^{k}, \oplus=+^{k}$, tensors the Weighted Constraint Satisfaction Problem


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## We always use $+^{k}$

The "local polytope" [Sch76; Kos99; Wer07]

$$
\begin{array}{cr}
\text { Minimize } \sum_{i, a} \varphi_{i}(a) \cdot x_{i a}+\sum_{\substack{\varphi_{i j \in \Phi} \in \Phi \\
a \in D^{j}, b \in D^{j}}} \varphi_{i j}(a, b) \cdot y_{i a j b} \text { such that } & \\
\sum_{a \in D^{i}} x_{i a}=1 & \forall i \in\{1, \ldots, n\} \\
\sum_{b \in D^{j}} y_{i a j b}=x_{i a} & \forall \varphi_{i j} \in \Phi, \forall a \in D^{i} \\
\sum_{a \in D^{i}} y_{i a j b}=x_{j b} & \forall \varphi_{i j} \in \Phi, \forall b \in D^{j} \\
x_{i a} \in\{0,1\} & \forall i \in\{1, \ldots, n\}
\end{array}
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$n d+e d^{2}$ variables, $n+2 e d$ constraints

1 Optimization

2 Algorithms

- Conditioning based: systematic and local search
- Elimination based: local consistency and variable elimination


## 3 All Toulbar2 bells and whistles

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| Conditioning: $\varphi_{S \mid X=a} \quad(X \in S)$ | Assignment |
| :--- | ---: |
| $\varphi_{S \mid X=a}(v)=\left(\varphi_{S}(v \cup\{X=a\})\right.$ | Scope $S-\{X\}$, negligible complexity |



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## Assignment

Scope $S-\{X\}$, negligible complexity

\[

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Conditioning by $X_{2}=b$


- If all $\left|D^{X}\right|=1$ obvious minimum update $k$ to $\Phi_{\mathcal{M}}(v)$
■ Else choose $X \in V$ s.t. $\left|D^{X}\right|>1$ and $u \in D^{X}$ and reduce to

1. one query where we condition by $X_{i}=u$
2. one where $u$ is removed from $D^{X}$

- Return the minimum


## Optimization

## Branch and Bound [LW66]

If the local lower bound reaches the global upper bound Prune!

## Partial search

Relaxed nruning $\left((1+\alpha) \varphi_{\varnothing} \geq k\right)$ [Poh70], bounded number of backtracks or discrepencies (LDS [HG95])

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Optimization
If the local lower bound, reaches the global upper bound

## Prune!

Partial search
Relaxed pruning $\left((1+\alpha) \varphi_{\varnothing} \geq k\right)$ [Poh70], bounded number of backtracks or discrepencies (LDS [HG95])

## Depth First (CP) or Best First (ILP)?

- Uses Depth-First Search for a bounded amount of backtracks
- Pending nodes are pushed onto a list of Open nodes
- The next DFS starts from the best Open node
- Tree-decomposition friendly (BTD [GSV06]/AND-OR search [MD09])


## Nice properties

- Cood' upper bounds quickly (DFS)
- A constantly improving lower bound (optimality gap)
- Implicit restarts, easy parallelization


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Improved: keep, reset $s$ to $s_{0}$
Else: forget, set $s$ to $s+1$

Combination of $\varphi_{S}$ and $\varphi_{S^{\prime}} \quad$ Space/time $O\left(d^{\mid S \cup S^{\prime}}\right)$ for tensors
$\left(\varphi_{S}+{ }^{k} \varphi_{S^{\prime}}\right)(v)=\varphi_{S}(v[S])+\varphi_{S^{\prime}}\left(v\left[S^{\prime}\right]\right)$


Elimination of $X \in S$ from $\varphi_{S}$
$\varphi_{s}\left[-X \backslash(u)=\min _{v \in D} \varphi_{s}(u \cup v)\right.$

Time $O\left(d^{|S|}\right)$, space $O\left(d^{|S|-1}\right)$ for tensors
Produces relaxations

Eliminate $X_{1}$
$\varnothing$
5

Combination of $\varphi_{S}$ and $\varphi_{S^{\prime}}$
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Elimination of $X \in S$ from $\varphi_{S}$ Time $O\left(d^{|S|}\right)$, space $O\left(d^{|S|-1}\right)$ for tensors $\varphi_{S}[-X](u)=\min _{v \in D^{X}} \varphi_{S}(u \cup v)$


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\varphi_{S}[-X](u)=\min _{v \in D^{X}} \varphi_{S}(u \cup v)
$$

Time $O\left(d^{|S|}\right)$, space $O\left(d^{|S|-1}\right)$ for tensors
Produces relaxations

Eliminate $X_{2}$
$X_{1}$
$5|6| 5$

Eliminate $X_{1}$

## Used together

- Combination accumulates all information in a single function
- Elimination forgets one variable without loosing optimality information


## At the core of

- I ocal consistencies, Unit propagation: subproblem induced by one function
- Variable elimination, the Resolution Principle: subproblem around one variable


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## At the core of

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## Arc consistency of $X_{i}$ w.r.t. $\varphi_{i j}$ [RBW06]

- Combine $\varphi_{i j}$ and the unary $\varphi_{j}$
- Eliminate $X_{j}$ producing a function (message) on $X_{i}$

$$
m_{i}^{j}=\left(\varphi_{i j}+\frac{k}{k} \varphi_{j}\right)\left[-X_{j}\right]
$$

## Properties

The message can be added to $\varphi_{i}$

- $X_{i}$ is AC w.r.t. $\varphi_{i j}$ if $m_{j}^{i} \leq \varphi_{i}$
$\square$ Unique fixpoint, reached in polynomial time
- Support of $u \in D^{i}$ on $D^{j}$
(relaxation, value deletion)
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## Obvious issue

Messages can not be included in the CFN: loss of equivalence, meaningless result

Equivalence Preserving Transformations with $-{ }^{k}\left(\alpha-{ }^{k} \beta\right) \equiv((\alpha=k)$ ? $k: \alpha-\beta)$

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$m_{1}^{2}$

$\Downarrow \quad m_{\varnothing}^{1}$

$$
\varphi_{\varnothing}=1
$$

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## The many "soft ACs" [Coo+10]

- NC: one unary function [Lar02]

Unary supports $\left(\varphi_{i}(u)=0\right)$

- +AC: one binary function [Sch00; Lar02]

Arc supports $\left(v \in D^{j}, \varphi_{i j}(u, v)=0\right)$

- +DAC: FDAC, binary \& unary function (+ direction) [Coo03]
- +Existential AC: EDAC, a star (variable incident functions) [Lar+05]
- +Virtual AC: any spanning tree [Coo+08; Coo+10]

Full Supports
EAC supports
VAC supports

## Properties

Related works in Comp. Vision [Kol06; Son+12; Wer07; Kol15]

- Proper extension of classical NC/DAC or AC respectively
- Polynomial time and $O(e d)$ space
- Incremental, strengthens $\varphi_{\varnothing}$
$(\mathrm{VAC} \geq \mathrm{EDAC} \geq \mathrm{FDAC} \geq \mathrm{AC} \geq \mathrm{NC})$
$\square$ May have several fixpoints $/ \varphi_{\varnothing}$


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Related works in Comp. Vision [Kol06; Son+12; Wer07; Kol15]

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$$
(k=1)
$$

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Sequence of integer EPTs
Computing a sequence of integer EPTs that maximizes $\varphi_{\varnothing}$ is decision NP-complete [CSO4]

Set of rational EPTs (OSAC [sch76; Cooo7; Wero7; Coot10])
Computing a set of rational EPTs maximizing $\varphi_{\varnothing}$ is in P , solvable by Linear Prog. +AC
Solving the dual of the local polytope +AC enforcing $(k)$

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Optimal Soft Arc Consistency (optimization alone)

## Variables for a binary CFN, no constraints [Sch76; Kos99; CGS07; Wer07; Coo+10]

1. $u_{i}$ : amount of cost shifted from $\varphi_{i}$ to $\varphi_{\varnothing}$
2. $p_{i j a}$ : amount of cost shifted from $\varphi_{i j}$ to $\varphi_{i}(a)$
3. $p_{j i b}$ : amount of cost shifted from $\varphi_{i j}$ to $\varphi_{j}(b)$

## OSAC



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## OSAC

$$
\begin{array}{lr}
\text { Maximize } & \sum_{i=1}^{n} u_{i} \\
& \varphi_{i}(a)-u_{i}+\sum_{\left(\varphi_{i j} \in C\right)} p_{i j a} \geq 0 \\
\varphi_{i j}(a, b)-p_{i j a}-p_{j i b} \geq 0 & \forall i \in\{1, \ldots, n\}, \forall a \in D^{i} \\
\text { subject to } \\
\end{array}
$$

The "local polytope"

$$
\text { Minimize } \sum_{i, a} \varphi_{i}(a) \cdot x_{i a}+\sum_{\substack{\varphi_{i j} \in \Phi \\ a \in D^{\prime}, b \in D^{j}}} \varphi_{i j}(a, b) \cdot y_{i a j b} \text { such that }
$$

$$
\begin{array}{lr}
\sum_{a \in D^{i}} x_{i a}=1 & \forall i \in\{1, \ldots, n\} \\
\sum_{b \in D^{j}} y_{i a j b}=x_{i a} & \forall \varphi_{i j} \in \Phi, \forall a \in D^{i} \\
\sum y_{i a j b}=x_{j b} & \forall \varphi_{i j} \in \Phi, \forall b \in D^{j}
\end{array}
$$

$u_{i}$ multiplier for (2), $p_{i j a} / p_{j b b}$ for (3) and (4)

## Problem solved by OSAC/VAC [Coo+10; KZ17]

- Tree-structured problems
- Permutated submodular problems
(eg. Min-Cut, Min/Max-closed relations)
$\square \mathrm{OSAC} / \mathrm{VAC}+\forall X_{i}, \exists!u \in D^{i}$ s.t. $\varphi_{i}(u)=0$

Supports provide value ordering heuristics
EAC supports $u$ for $X_{i}: \varphi_{i}(u)=0$, can be extended for free on $X_{i}$ 's star

- VAC supports can be extended for free on any spanning tree [Kol06; Coo+08; Coo+10]

NC provides cost-based pruning

$$
\text { If }\left(\varphi_{\varnothing}+\varphi_{i}(u)\right)=k, \text { NC deletes } u
$$

Local consistencies vs. LP

- OSAC empirically very expensive to enforce
- Local consistencies provide fast approximate LP bounds
- and deal with constraints seamlessly


## CFN Local Consistencies

Fnhance CP with fast incremental approximate Linear Programming dual bounds

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Enhance CP with fast incremental approximate Linear Programming dual bounds

## 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.

## Kind words from OpenGM2 developpers

"ToulBar2 variants were superior to CPLEX variants in all our tests"[HSS18]

## VAC vs. LP on Protein design problems

## CPLEX V12.4.0.0

Problem '3e4h.LP' read.
Root relaxation solution time $=811.28 \mathrm{sec}$.

MIP - Integer optimal solution: Objective $=150023297067$
Solution time $=864.39 \mathrm{sec}$.

## tb2 and VAC

loading CFN file: 3e4h.wcsp
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## Kind words from OpenGM2 developpers

"ToulBar2 variants were superior to CPLEX variants in all our tests"[HSS18]

- combination and elimination are Ok
- but subtracting a clause from another clause does not yield a clause (CNF/DNF)
- generates additional "compensation" clauses [LH05; HLO07; BLM07; LHG08])


## Variable elimination

## Definition (Message from $X$ to its neighbors)

Let $X \in V$, and $\Phi^{X}$ be the set $\left\{\varphi_{S} \in \Phi\right.$ s.t. $\left.X \in S\right\}, T$, the neighbors of $X$.
The message $m_{T}^{\Phi X}$ from $\Phi^{X}$ to $T$ is:

$$
m_{T}^{\Phi_{X}}=\left(\sum_{\varphi_{S} \in \Phi^{X}}^{k} \varphi_{S}\right)[-X]
$$

The message contains all the effect of $X$ on the optimization problem Distributivity


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Daoopt \& mini-buckets [DR03] split $\Phi^{X}$ in subsets of controlled size (lower bound)



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## On the fly Variable elimination

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1 Optimization
2 Algorithms

3 All Toulbar2 bells and whistles
4 Learning CFN from data

Additional algorithmic ingredients

- Variable ordering: weighted degree [Bou+04], last conflict [Lec+09], VAC-based [TGK20]
- Value ordering (for free): existential or virtual supports
- Dominance analysis (substitutability/DEE) [Fre91; DPO 13; All+14]
- Function decomposition [Fav+11]
- Global cost functions (weighted Regular, All-Diff, Among...) [LL12; All+16]
$\square$ Incremental solving, guaranteed diverse solutions [Ruf+ 19]
- Parallel decomposed Variable Neighborhood Search/LDS (UPDGVNS [Oua+20])

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## Practical aspects

- C++ Open source, MIT licence on GitHub, available in Debian
- Uses 64 bits integer costs to represent adjustable precision decimal costs
- Tackles minimization, maximization with costs of arbitrary signs and constraints
- JSON compatible CFN input format
- Python API (PyToulbar2)


## 3026 instances of various origins

■ MRF: Probabilistic Inference Challenge 2011

- CVPR: Computer Vision \& Pattern Recognition OpenGM2
- CFN: Cost Function Library
- MaxCSP: MaxCSP 2008 competition
- WPMS: Weighted Partial MaxSAT evaluation 2013
- CP: MiniZinc challenge 2012/13

| Benchmark | Nb. | UAI | WCSP | LP(direct) | LP(tuple) | wCNF(direct) | wCNF(tuple) | MINIZINC |
| :--- | :---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| MRF | 319 | 187 MB | 475 MB | 2.4 G | 2.0 GB | 518 MB | 2.9 GB | 473 MB |
| CVPR | 1461 | 430 MB | 557 MB | 9.8 GB | 11 GB | 3.0 GB | 15 GB | $\mathrm{~N} / \mathrm{A}$ |
| CFN | 281 | 43 MB | 122 MB | 300 MB | 3.5 GB | 389 MB | 5.7 GB | 69 MB |
| MaxCSP | 503 | 13 MB | 24 MB | 311 MB | 660 MB | 73 MB | 999 MB | 29 MB |
| WPMS | 427 | $\mathrm{~N} / \mathrm{A}$ | 387 MB | 433 MB | $\mathrm{N} / \mathrm{A}$ | 717 MB | $\mathrm{N} / \mathrm{A}$ | 631 MB |
| CP | 35 | 7.5 MB | 597 MB | 499 MB | 1.2 GB | 378 MB | 1.9 GB | 21 KB |
| Total | 3026 | 0.68 G | 2.2 G | 14 G | 18 G | 5 G | 27 G | 1.2 G |




Optimality gap of the Simulated annealing solution as problems get harder


DWave approximations
within 1.16 of optimum, $10 \%$ of the time
$4.35,50 \%$ of the time
$8.45,90 \%$ of the time

| toulbar2 |
| :---: | :---: | :---: | :---: | :---: |
| cplex |
| UDGVNS |




1 Optimization

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4 Learning CFN from data

## Definition (Learning a pairwise CFN from high quality solutions)

Given:

- a set of variables $V$,
- a set of assignments $\boldsymbol{E}$ i.i.d. from an unknown distribution of high-quality solutions

Find a pairwise CFN $\mathcal{M}$ that can be solved to produce high-quality solutions

MRFs tightly connected to CFNs $(k=\infty)$
$\longrightarrow$

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MRFs tightly connected to CFNs $(k=\infty)$
(additive energy)
MRF M $\underset{-\log (x)}{ } \quad$ CFN M $^{\ell} \xrightarrow[\exp (-x)]{ } \quad$ MRF M

## Opens the door to learning from data $\boldsymbol{E}$

- $E$ a set of i.i.d. assignments of $V$
- The $\log$-likelihood of $\mathcal{M}$ given $\boldsymbol{E}$ is $\log \left(\prod_{v \in E} P_{\mathcal{M}}(v)\right)=\sum_{v \in E} \log \left(P_{\mathcal{M}}(v)\right)$
- Maximimizing loglikelihood over all binary $\mathcal{M}$

$$
\left(O\left(\frac{n(n-1)}{2} d^{2}\right) \text { costs }\right)
$$

## Maximum $\log$ likelihood $\mathcal{M}$ on $\mathcal{M}_{\ell}$



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$$

Maximum $\log$ likelihood $\mathcal{M}$ on $\mathcal{M}_{\ell}$

$$
\begin{aligned}
\mathcal{L}(\mathcal{M}, \boldsymbol{E}) & =\log \left(\prod_{v \in E} P_{\mathcal{M}}(v)\right)=\sum_{v \in E} \log \left(P_{\mathcal{M}}(v)\right) \\
& =\underbrace{}_{\text {-costs of } E \text { samples }} \underbrace{}_{\text {Soft-Min of all assignment costs }} \\
= & \sum_{v \in E}\left(-C_{\mathcal{M}^{e}}(v)\right)
\end{aligned}
$$

## Learning a Cost Function Network from high-quality solutions



## Learning a Cost Function Network from high-quality solutions


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