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Constraint and Cost Function Networks: feasibility, optimization and learning.

Thomas Schiex

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CONSTRAINT & COST FUNCTION NETWORKS: FEASIBILITY, OPTIMIZATION AND LEARNING

JFPC'2021



T. SCHIEX (AND PLENTY OF COLLEAGUES)

UNIVERSITÉ FÉDÉRALE DE TOULOUSE, ANITI, INRAE MIAT, TOULOUSE, FRANCE

JUNE 22, 2021



A Constraint Network $\langle \mathbf{V}, \Phi \rangle$

- a sequence of discrete domain variables \mathbf{V}
- a set Φ of e Boolean functions (or constraints)
- Each $\varphi_S \in \Phi$ is a truth function from $D^S \rightarrow \{t, f\}$

Joint truth function

$$\Phi_{\mathcal{M}} = \bigwedge_{\varphi_S \in \Phi} \varphi_S$$

The Constraint Satisfaction Problem (NP-complete)

- Is it possible to make $\Phi_{\mathcal{M}} = t$?

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Languages for domains and constraints

- Constraint Networks: Boolean tables (tensors) for domains and constraints
- Constraint Programming: interval variables, specialized constraints, control

Tables (or tensors) for φ_S

- A multidimensional table with a Boolean for every tuple in D^S
- Says if it is authorized (t) or not (f)

Pairwise difference (3 values)

$$\begin{bmatrix} f & t & t \\ t & f & t \\ t & t & f \end{bmatrix}$$

Languages for domains and constraints

- Constraint Networks: Boolean tables (tensors) for domains and constraints
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Global constraints

- Names for specific (useful) constraints

Most famous

`ALLDIFFERENTS`

Languages for domains and constraints

- Constraint Networks: Boolean tables (tensors) for domains and constraints
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Application domains: NP and beyond

Excel at the analysis of complex perfectly known systems

Digital circuit verification, scheduling and other resource management problems, planning, software verification, theorem proving,...

Biology?

Cost Function Network $\langle \mathcal{V}, \Phi, k \rangle$

- a sequence of discrete domain variables \mathcal{V}
- a set Φ of e integer cost functions
- Each $\varphi_S \in \Phi$ is a numerical function bounded by k (finite or infinite)

Joint cost function using $a +^k b = \min(a + b, k)$

$$\Phi_{\mathcal{M}} = \sum_{\varphi_S \in \Phi}^k \varphi_S$$

The Weighted Constraint Satisfaction Problem (decision NP-complete)

- What is the minimum of $\Phi_{\mathcal{M}}$?

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Global functions

- Names for specific (useful) functions

Soft difference (3 values)

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

A useful one

KNAPSACK_S

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Costs and constraints

- We assume non negative integer costs
- A constraint is a cost function that maps to $\{0, k\}$
- $k = 1$ defines a pure Constraint Network

Optimum preserving operations

- scaling: $2^{63} \approx 19$ digits. Fixed decimal point numbers ok
- shifting: negative numbers and maximization ok

Extra assumptions inside the solver

w/o l.o.g.

- CFNs have all unary functions $\varphi_i, X_i \in \mathcal{V}$
- CFNs have a constant function φ_\emptyset

(domains)

Crucial property

 φ_\emptyset is a lower bound of the joint function $\Phi_{\mathcal{M}}$

EXAMPLE: MIN-CUT

Graph $G = (V, E)$ with edge weight function w

- A Boolean variable X_i per vertex $i \in V$
- A cost function per edge $e = (i, j) \in E : \varphi_{ij} = w(i, j) \times \mathbb{1}[x_i \neq x_j]$

A simple graph

- vertices $\{1, 2, 3, 4\}$
- cut weight 1 or 1.5 (1, 3)
- edge (1, 2) hard

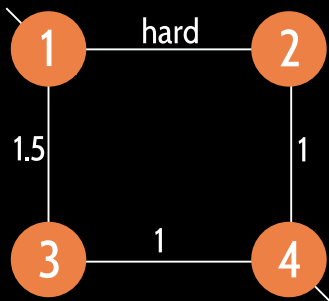
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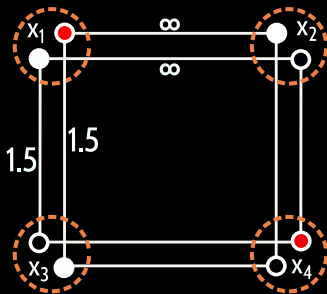
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- cut weight 1 or 1.5 (1, 3)
- edge (1, 2) hard



Min-CUT on 4 variables

```
{
  "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": [0.0,1.5,1.5,0.0]},
    "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]}
  }
}
```

Min-CUT on 4 variables

```
import pytoulbar2
myCFN = pytoulbar2.CFN(100,1) # ub, resolution (optional)
for i in range(4):
    myCFN.AddVariable("x"+str(i+1),["l", "r"]) # returns an index
myCFN.AddFunction(["x1"], [0,100])
myCFN.AddFunction(["x4"], [100,0])
myCFN.AddFunction(["x1","x3"], [0,1.5,1.5,0])
...
sol = myCFN.Solve() # returns a triple (sol, cost, _)
```


Definition

- Variables X_{ij} for cell (i, j) has domain $\{1, \dots, 9\}$
- Set R_i (resp. C_j) contains all variables of row i (resp. column j)
- Set S_i contains all variables in sub-cell i
- There is an ALL-DIFFERENT constraint on each of these
- or a clique of pairwise DIFFERENT constraints

Example

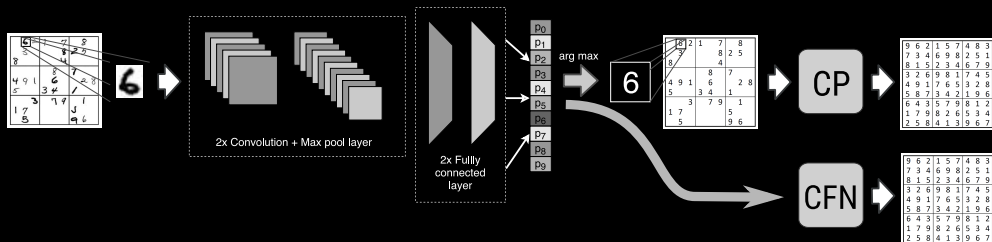
Let's have a look at the `pytoulbar2` code.

```
myCFN = pytoolbar2.CFN(1)    # k = 1, so CSP

for i in range(9):
    for j in range(9):
        vIdx = myCFN.AddVariable("X"+str(i+1)+"."+str(j+1),range(1,10))
        columns[j].append(vIdx)
        rows[i].append(vIdx)
        cells[(i//3)*3+(j//3)].append(vIdx)

for scope in rows+columns+cells:
    addCliqueAllDiff(myCFN,scope)    # Adds a clique of pairwise difference

for v,h in enumerate(grid):
    if h: myCFN.AddFunction([v],[0 if i == h else 1 for i in range(1,10)])
```



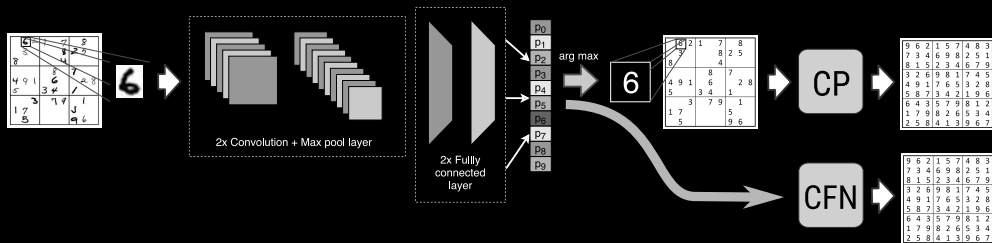
The Boolean way

Thanks to Tias Gun for the picture above

1. Assign the cell variable with the prediction
2. LeNet has 99.2% accuracy, SAT-Net dataset 36.2 hints (avg):74.7% max. accuracy

The Numbers way

1. Add LeNet output tensor (negated) as a cost function
2. $(\min \sum -\log) \equiv (\max \prod)$ probabilities >99% acc.



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```
myCFN = pyoulbar2.CFN(1000000,6)

for i in range(9):
    for j in range(9):
        vIdx = myCFN.AddVariable("X"+str(i+1)+"."+str(j+1),range(1,10))
        columns[j].append(vIdx)
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for scope in rows+columns+cells:
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for v, h in enumerate(grid):
    if h: myCFN.AddFunction([v],-MNIST_output(csol,v,h))
```

CFN compared to a COP approach¹

- COP (OR-Tools) + global All-Different
- CFN (toulbar2) + pairwise differences

Tight links with (I)LP

Let's look at the primal connection

¹Maxime Mulamba et al. “Hybrid Classification and Reasoning for Image-based Constraint Solving”. In: *Proc. of CPAIOR'20, also in arXiv preprint arXiv:2003.11001*. 2020, pp. 364–380.

CFN compared to a COP approach¹

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- CFN (toulbar2) + pairwise differences 0.05"
- 99.6% of all problems are solved backtrack-free by toulbar2
- CFN bounds way tighter than COP bounds [LL12]

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The “local polytope” [Sch76; Kos99; Wer07]

(without eq. (1))

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

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

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

$$\sum_{a \in D^i} y_{iajb} = x_{jb} \quad \forall \varphi_{ij} \in \Phi, \forall b \in D^j$$

$$x_{ia} \in \{0, 1\} \quad \forall i \in \{1, \dots, n\} \quad (1)$$

$nd + ed^2$ variables, $n + 2ed$ constraints: a strong but expensive bound

- 1 Systematic search and local search
- 2 Pruning and Bounds
- 3 All Toulbar2 bells and whistles
- 4 WCSP solving has made huge progress
- 5 Learning CFN from data

Systematic tree search

Time $O(d^n)$, linear space

- If all $|D^X| = 1$ obvious minimum
- Else choose $X \in V$ s.t. $|D^X| > 1$ and $u \in D^X$ and reduce to
 1. one query where we set $X = u$
 2. one where u is removed from D^X
- Return the minimum

update k to $\Phi_{\mathcal{M}}(v)$

Optimization

Branch and Bound [LW66]

If the $\underbrace{\text{local lower bound}}_{\varphi_0}$ reaches the $\underbrace{\text{global upper bound}}_k$

Prune!

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DEPTH FIRST (CP) OR BEST FIRST (ILP)?

Hybrid Best First Search [All+15]

Anyspace

- 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

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

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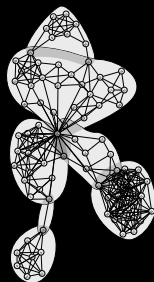
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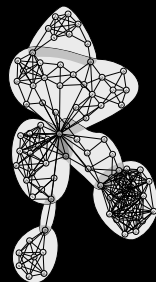
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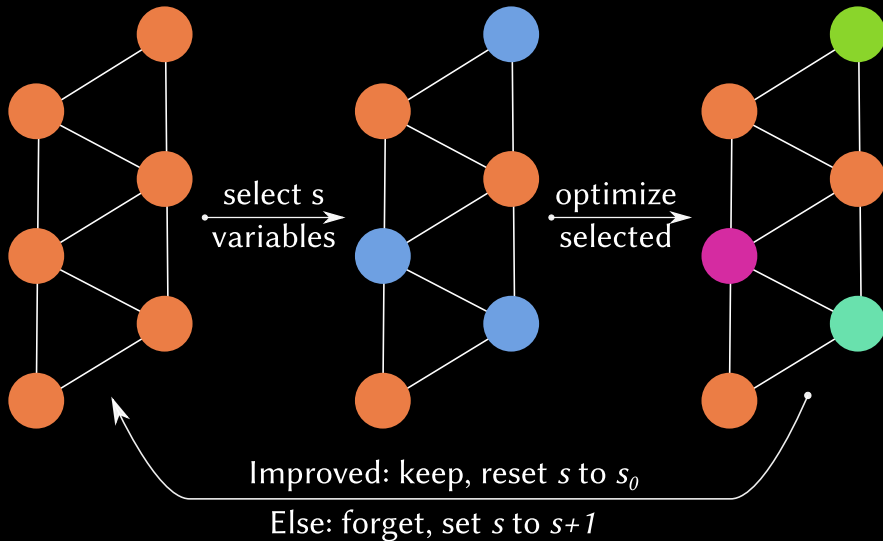
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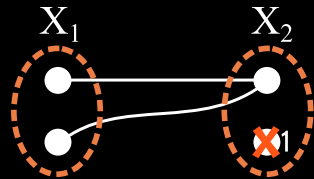
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Filtering by Arc Consistency (support)

A value $u \in D^i$ with no value $v \in D^j$ such that $\varphi_{ij}(u, v) = 0$ can be deleted, leaving the problem equivalent.



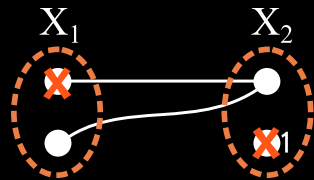
Properties

- Combine φ_{ij} and φ_j
- Project on X_i
- Combine with φ_i
- Unique fixpoint (monotonic), polynomial time

(inconsistency detection)

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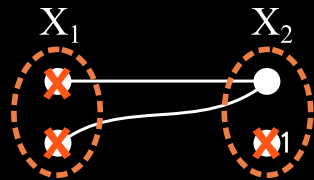
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Obvious issue

One cannot add functions to the CFN: loss of equivalence, meaningless result

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

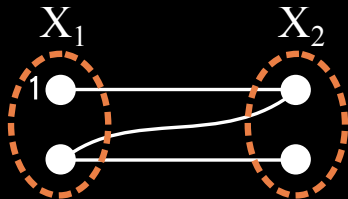
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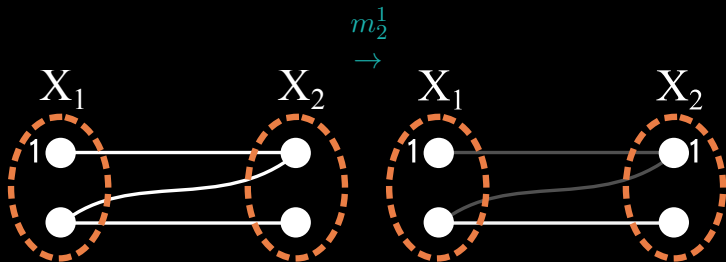
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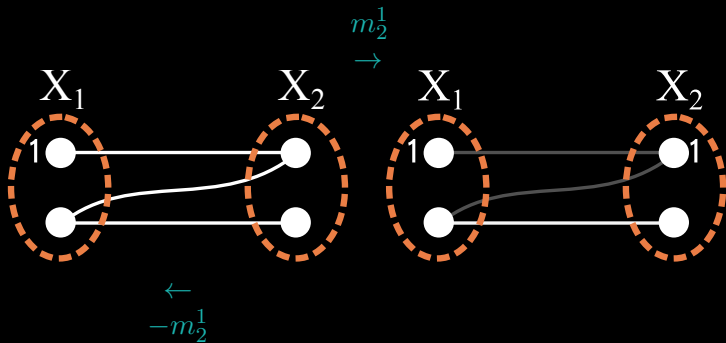
(Loss of) properties

Preserves equivalence but non-monotonic and fixpoints may be non unique (or may not exist)



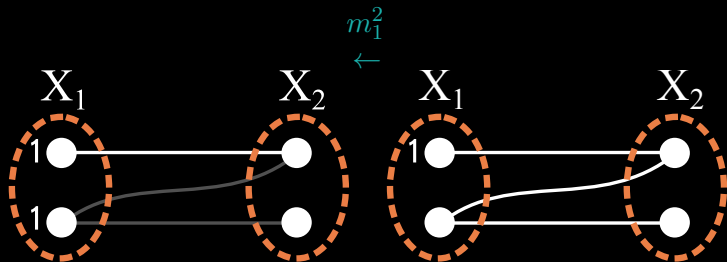
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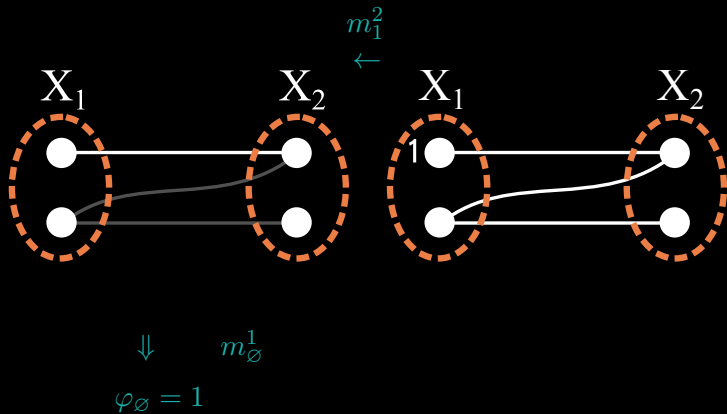
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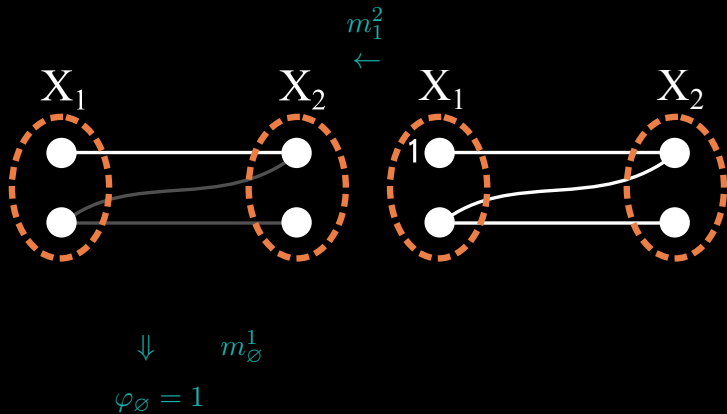
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The many “soft ACs”

One paper to read: [Coo+10]

- NC+AC+DAC (FDAC): binary & unary (+ direction)[Sch00; Lar02; Coo03] Full Supports
- +Existential AC: EDAC, a star (variable incident functions) [Lar+05] EAC supports
- +Virtual AC: any spanning tree [Coo+08; Coo+10] VAC supports

Supports provide value ordering heuristics

- EAC: $\varphi_i(u) = 0$ can be extended for free on X_i 's star
- VAC: $\varphi_i(u) = 0$ can be extended for free on any spanning tree [Kol06; Coo+08; Coo+10]

NC provides reduced cost-based pruning (back-propagation)

If $(\varphi_\emptyset \stackrel{k}{+} \varphi_i(u)) = k$, NC deletes u

The many “soft ACs”

One paper to read: [Coo+10]

- NC+AC+DAC (FDAC): binary & unary (+ direction)[Sch00; Lar02; Coo03] Full Supports
- +Existential AC: EDAC, a star (variable incident functions) [Lar+05] EAC supports
- +Virtual AC: any spanning tree [Coo+08; Coo+10] VAC supports

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Properties

- Proper extension of classical NC/DAC or AC respectively ($k = 1$)
- Polynomial time, $O(ed)$ space (Generalized ACs)
- Incremental, strengthens φ_\emptyset ($\text{NC} \leq \text{AC} \leq \text{FDAC} \leq \text{EDAC} \leq \text{VAC}$)
- Stronger bounds than AC in COP [LL12]

Set of rational EPTs

OSAC [Sch76; Coo07; Wer07; Coo+10]

Maximizing φ_\emptyset is in P (local polytope dual + AC for 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 φ_i to φ_\emptyset
2. p_{ija} : amount of cost shifted from φ_{ij} to $\varphi_i(a)$
3. p_{jib} : amount of cost shifted from φ_{ij} to $\varphi_j(b)$

OSAC

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

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Problems solved [Coo+10; KZ17]

- Tree-structured problems
- Permuted submodular problems (e.g. Min-Cut)

OSAC empirically too expensive compared to VAC

- CFN Arc consistencies provide fast approximate LP bounds
- and deal with constraints seamlessly

CFN Local Consistencies

Enhance CP with fast incremental approximate Linear Programming dual bounds

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- 4 WCSP solving has made huge progress
- 5 Learning CFN from data

Additional algorithmic ingredients

- Value ordering (for free): existential or virtual supports
- Variable ordering: weighted degree [Bou+04], last conflict [Lec+09], VAC-based [TKK20]
- (On the fly) variable elimination [Lar00]
- Dominance analysis (substitutability/DEE) [Fre91; Des+92; DPO13; All+14]
- Function decomposition [Fav+11]
- Some global cost functions (weighted Regular, All-Diff, Among...) [LL12; All+16]
- Incremental solving, guaranteed diverse solutions [Ruf+19]
- Unified (Parallel) Decomposition Guided VNS/LDS (UPDGVNS [Oua+20])

More information

github.com/toulbar2/toulbar2

miat.inrae.fr/toulbar2

- 1 Systematic search and local search
- 2 Pruning and Bounds
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- 4 **WCSP solving has made huge progress**
- 5 Learning CFN from data

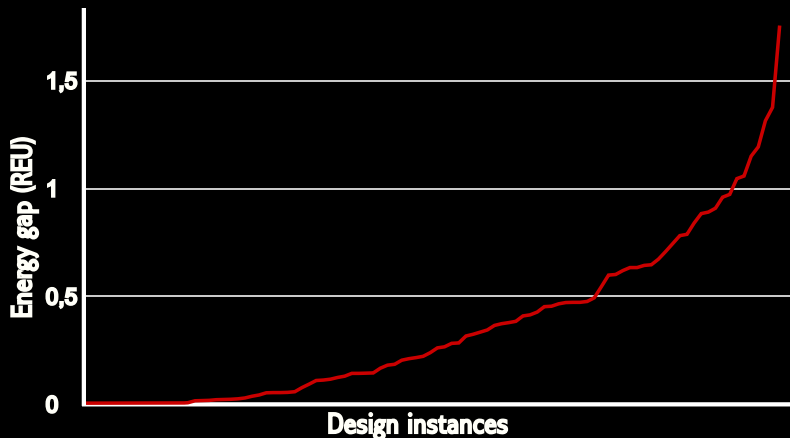
CPLEX V12.4.0.0

```
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

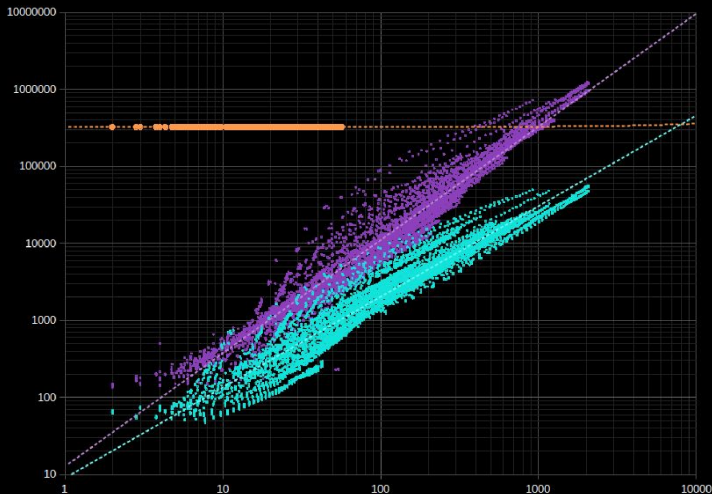
(AC3 based)

```
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.
```



Optimality gap of the Simulated annealing solution as problems get harder

²David Simoncini et al. “Guaranteed Discrete Energy Optimization on Large Protein Design Problems”. In: *Journal of Chemical Theory and Computation* 11.12 (2015), pp. 5980–5989. doi: 10.1021/acs.jctc.5b00594.



DWave approximations

kcal/mol

gap > 1.16 90% of the time

> 4.35, 50% of the time

> 8.45, 10% of the time

Kind words from Protein Designers³

The Toulbar[2] package for WCSPs significantly improved the state-of-the-art efficiency for protein design in the discrete pairwise model.

Kind words from OpenGM2 developpers (image processing)

“ToulBar2 variants were superior to CPLEX variants in all our tests”⁴

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Data mining, bioinformatics

Given a matrix of arbitrary real numbers, find a subset C of columns and R of rows such that the sum of numbers in the submatrix is maximized.

Dedicated global constraint

Presented in [BSD17; Der+19], dominates MILP and MIQCP.

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```
def generate_model(path):
    m = pandas.read_csv(path, sep='\t', header=None)
    r, c = m.shape
    model = pytoulbar2.CFN(100000, 10, True)
    for i in range(r):
        model.AddVariable("R"+str(i), ["out", "in"])
    for j in range(c):
        model.AddVariable("C"+str(j), ["out", "in"])
    for i in range(r):
        for j in range(c):
            model.AddFunction(["R"+str(i), "C"+str(j)], [0.0, 0.0, 0.0, -m[j][i]])
    return model

(solution, cost, _) = generate_model(sys.argv[1]).Solve()
```

The Global Constraint author

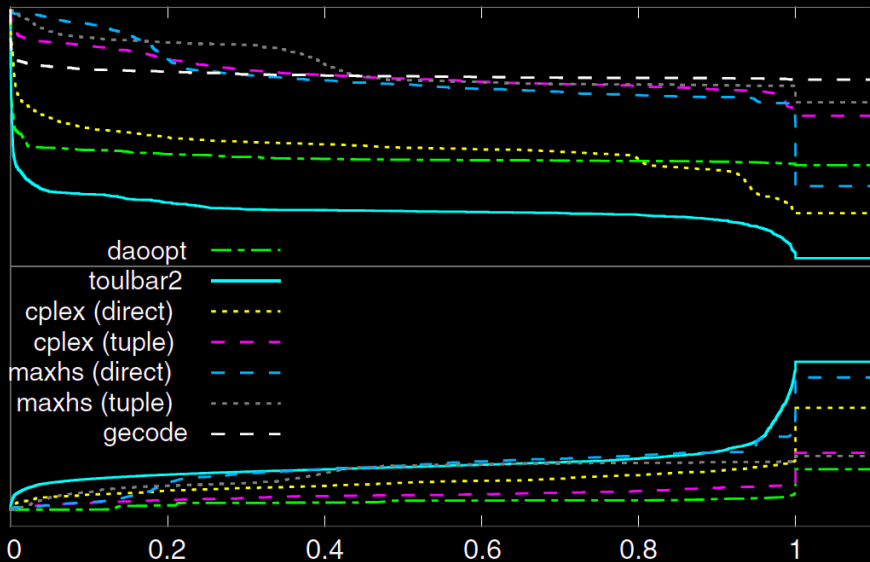
Je n'ai pas vraiment trouvé de cas [...] défavorable pour toulbar2.

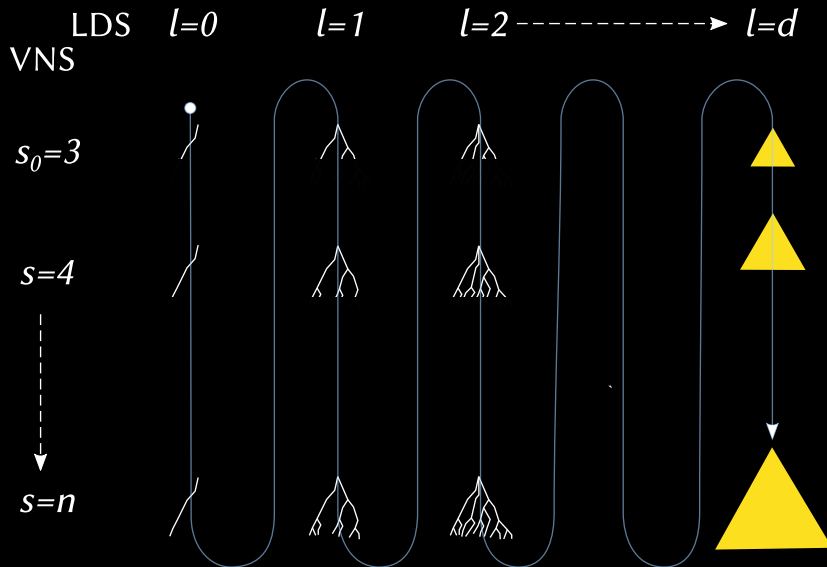
3026 instances of various origins

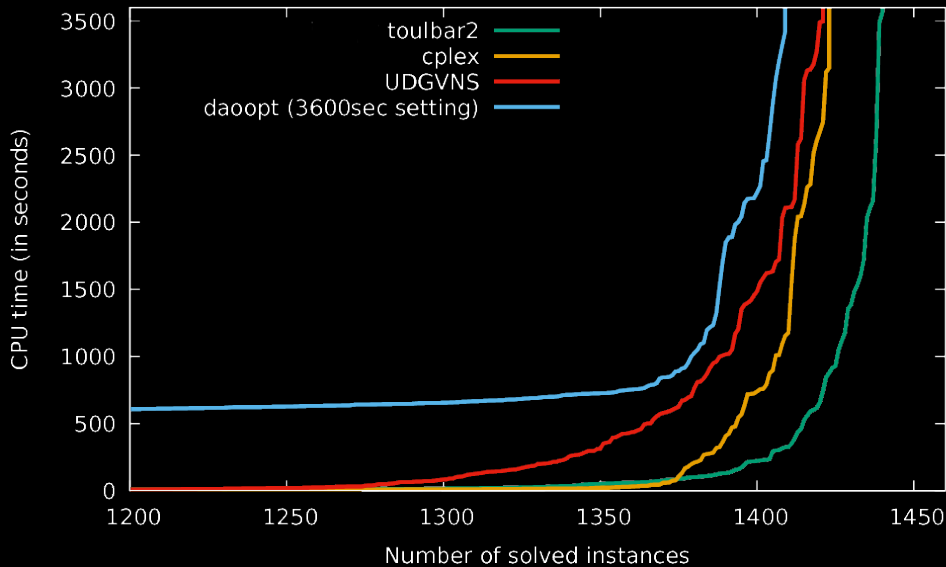
genoweb.toulouse.inra.fr/~degivry/evalgm

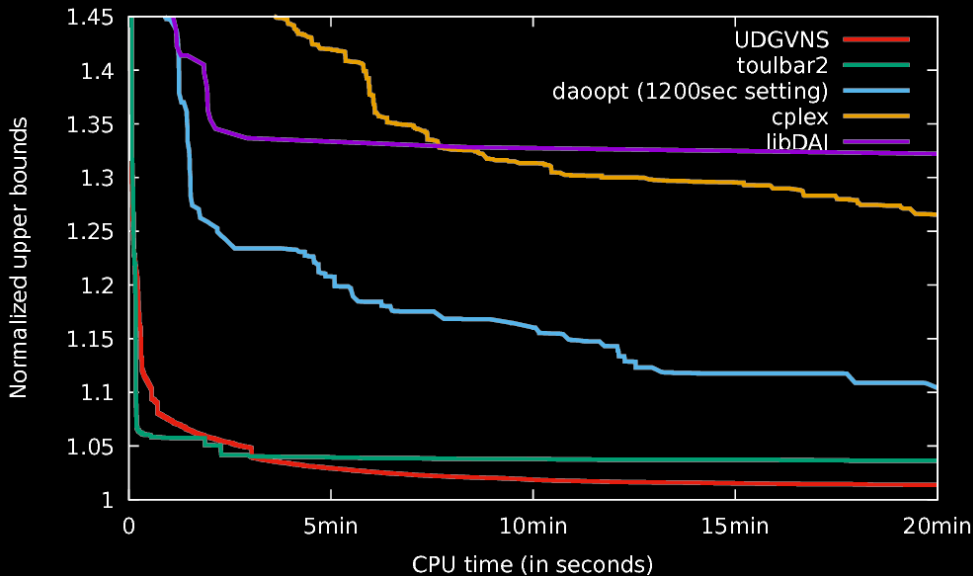
- MRF: Probabilistic Inference Challenge 2011
- CVPR: Computer Vision & Pattern Recognition OpenGM2
- CFN: Cost Function Library (CELAR, SPOT5, bioinformatics)
- MaxCSP: MaxCSP 2008 competition
- WPMS: Weighted Partial MaxSAT evaluation 2013
- CP: MiniZinc challenge 2012/13 (decomposable)

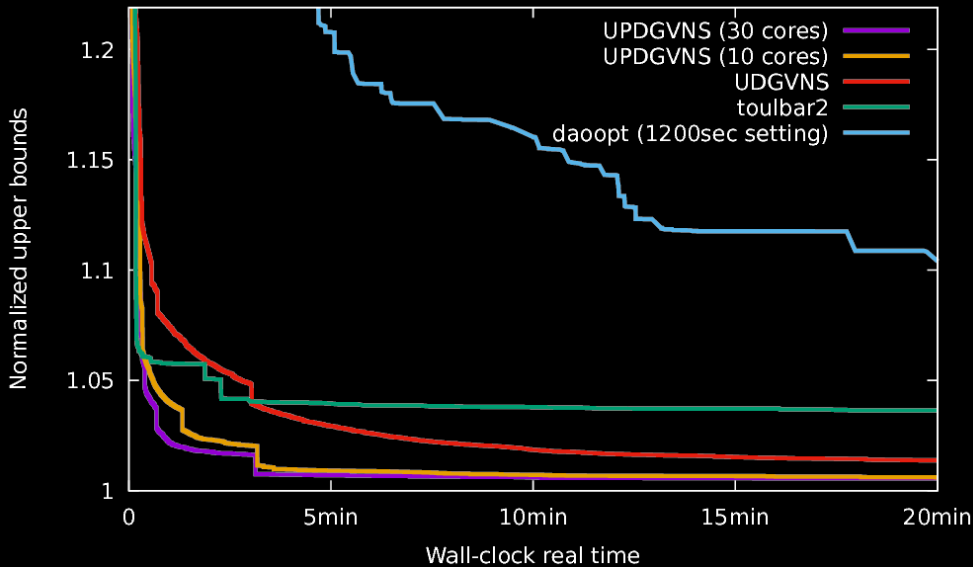
Benchmark	Nb.	UAI	WCSP	LP(direct)	LP(tuple)	WCNF(direct)	WCNF(tuple)	MINIZINC
MRF	319	187MB	475MB	2.4G	2.0GB	518MB	2.9GB	473MB
CVPR	1461	430MB	557MB	9.8GB	11GB	3.0GB	15GB	N/A
CFN	281	43MB	122MB	300MB	3.5GB	389MB	5.7GB	69MB
MaxCSP	503	13MB	24MB	311MB	660MB	73MB	999MB	29MB
WPMS	427	N/A	387MB	433MB	N/A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











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Definition (Learning a pairwise CFN from high quality solutions)

Given:

- a set of variables V ,
- a set of assignments 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

WHAT DOES LEARNING A CFN MEANS EXACTLY?

We use the language of pairwise tensors/tables

- There are at most $\frac{n(n-1)}{2}$ pairwise functions $\frac{81 \times 80}{2} = 3240$
- Each with $|D^i| \times |D^j|$ costs in \mathbb{R} (differentiability) 81
- For the Sudoku, 262,440 parameters to learn.

Maximum likelihood estimation

- E a set of i.i.d. assignments of V
- Interpret costs as energies ($\propto -\log(\text{probabilities})$)
- Maximize the probability of observing the samples in E

Maximum loglikelihood \mathcal{M} on \mathcal{M}_ℓ

$$\begin{aligned}
 \mathcal{L}(\mathcal{M}, E) &= \log\left(\prod_{v \in E} P_{\mathcal{M}}(v)\right) = \sum_{v \in E} \log(P_{\mathcal{M}}(v)) \\
 &= \sum_{v \in E} \log(\Phi_{\mathcal{M}}(v)) - \log(Z_{\mathcal{M}}) \\
 &= \underbrace{\sum_{v \in E} (-C_{\mathcal{M}^\ell}(v))}_{\text{-costs of } E \text{ samples}} - \underbrace{\log\left(\sum_{t \in \prod X \in V D^X} \exp(-C_{\mathcal{M}^\ell}(t))\right)}_{\text{Soft-Min of all assignment costs}}
 \end{aligned}$$

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 \end{aligned}$$

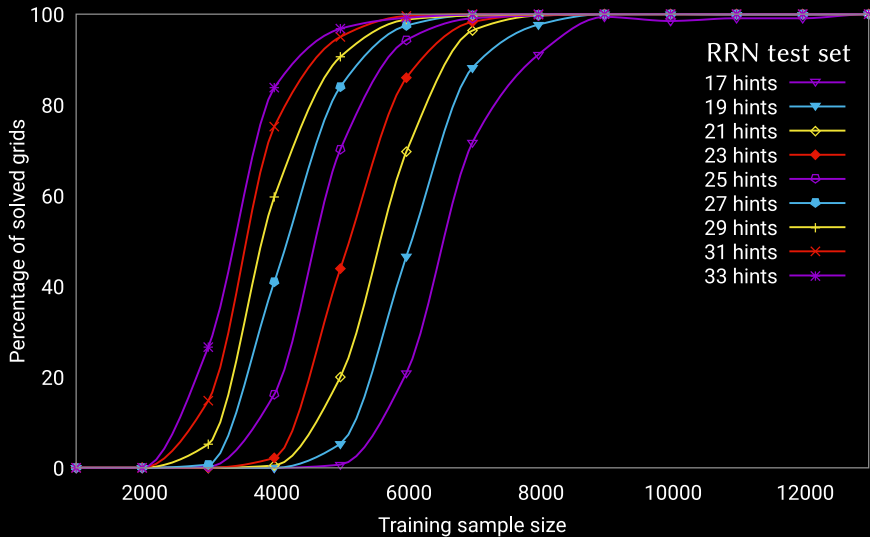
Algorithms and data-sets

- PE-MRF [Par+17] with L1-norm Regularization
- Validation set from the SAT-Net paper⁵ (36.2 hints)
- Validation set from the RRN paper⁶ with 17-34 hints.

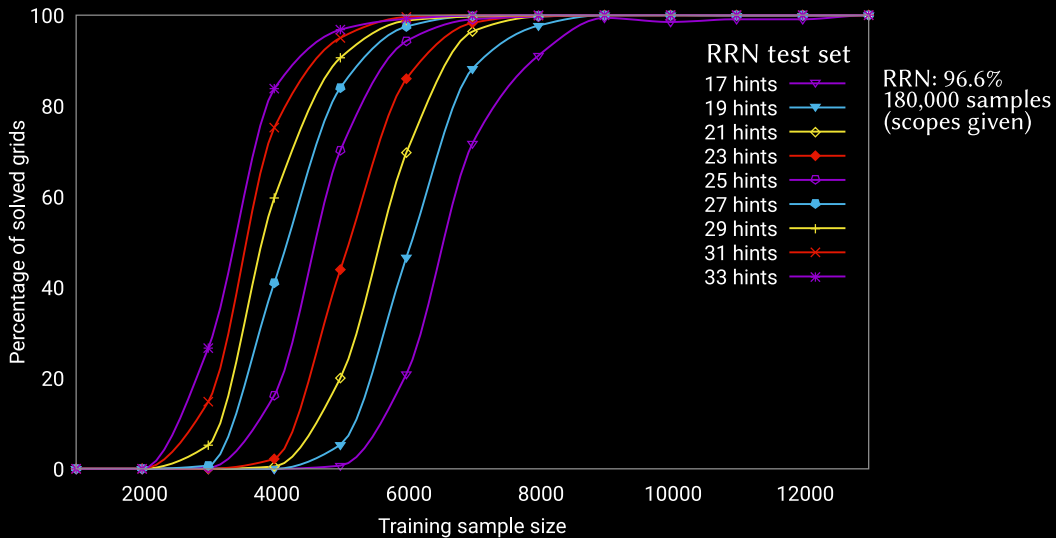
⁵Po-Wei Wang et al. “SATNet: Bridging deep learning and logical reasoning using a differentiable satisfiability solver”. In: *ICML '19 proceedings, arXiv preprint arXiv:1905.12149*. 2019.

⁶Rasmus Palm, Ulrich Paquet, and Ole Winther. “Recurrent relational networks”. In: *Advances in Neural Information Processing Systems*. 2018, pp. 3368–3378.

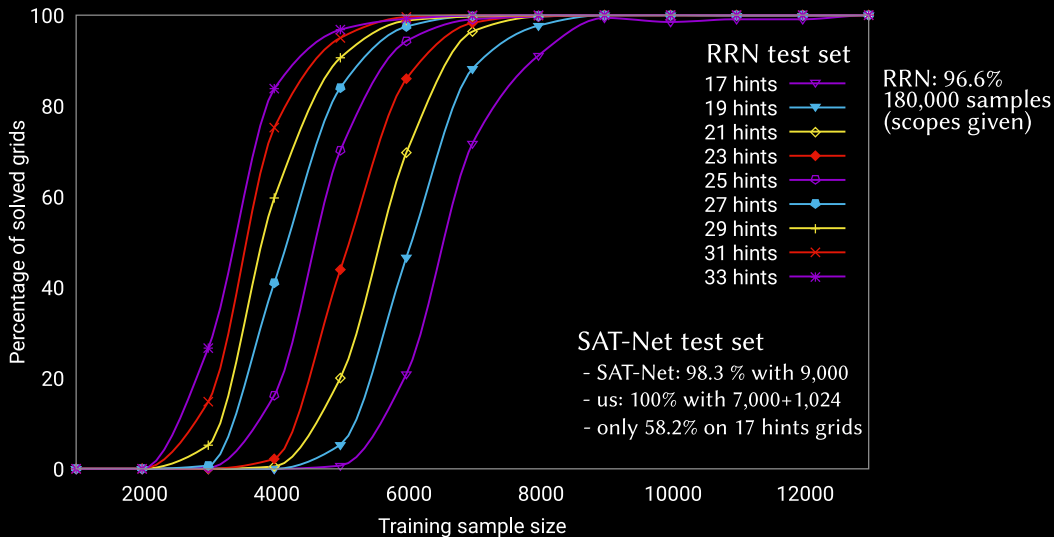
LEARNING HOW TO SOLVE THE SUDOKU



LEARNING HOW TO SOLVE THE SUDOKU



LEARNING HOW TO SOLVE THE SUDOKU



Learning from uncertain DL output is possible

- LeNet has 99.2% accuracy on handwritten digits
- Argmax decoding: 74.7% of the learning data-set would be incorrect
- Important to accept probabilistic information as input (PE-MRF)

Comparing with SAT-Net

- SAT-Net (9,000 samples):63.2%
- Toulbar2+PE-MRF (8,000+1,024 samples):76.3%

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NOT ONLY SUDOKUS OF COURSE...

See our CP2020 paper⁷

We show how it can learn user preferences and combine them with configuration constraints on Renault dataset (thanks to H. Fargier (IRIT)).

⁷Céline Brouard, Simon de Givry, and Thomas Schiex. “Pushing data into CP models using Graphical Model Learning and Solving”. In: *Principles and Practice of Constraint Programming–CP 2020*. Springer, 2020.

CFN/WCSP solving has made important progress

- Fast approximate LP-bounds (tighter than COP) subsuming AC
- Free value ordering heuristics
- Reduced-cost-based filtering (cost backpropagation)
- Structure aware search with improving optimality gap

CFN can be learned from data and combined with constraints

- Shares with ILP the capacity of dealing with fine grained numerical information
- Tractable learning with probabilistic input (DL/ML connection)
- With the (adjustable) power of (exact) solvers

Directions for improvement

- Global cost function and non monotonicity
- Interval variables and “arithmetic” filtering
- Unify CFN and COP: cost variables, multiple criteria
- Stronger incremental bounds
- Parallel search, conflict learning
- Try to minimize average tardiness in scheduling
- Improve CFN learning (sample size, (global) constraints)
- ...

THANK YOU ALL FOR YOUR ATTENTION!

And to all CFN/toulbar2 contributors

S. de Givry (INRAE)	G. Katsirelos (INRAE)	M. Zytnicki (PhD, INRAE)
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P. Jégou (LSIS)	A. Ouali (GREYC)	Y. Lebbah (GREYC)
L. Loukil (GREYC)	P. Boizumault (GREYC)	Mario (CU. Hong-Kong)
M. Lemaître (CERT)	L. Lobjois (CERT)	B. Hurley (Insight)
B. Neveu (INRIA, Sophia)	G. Trombettoni (INRIA)	...

Questions?

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