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

Thomas Schiex

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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 $\langle V, \Phi \rangle$

- a sequence of discrete domain variables 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)

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

From CSP to CP

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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

AllDifferent$_S$

From CSP to CP

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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 $\langle \boldsymbol{V}, \Phi, k \rangle$

- a sequence of discrete domain variables $\boldsymbol{V}$
- 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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- A multidimensional table with a number for every tuple in D^S

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

$\textsc{Knapsack}_S$

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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 $\varphi_i, X_i \in \boldsymbol{V}$ (domains)
- CFNs have a constant function $\varphi_\varnothing$

Crucial property

$\varphi_\varnothing$ is a lower bound of the joint function $\Phi_{\mathcal{M}}$

Example: Min-Cut

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 $e = (i, j) \in E : \varphi_{ij} = w(i, j) \times \mathbb{1}[x_i \neq x_j]$

A simple graph

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

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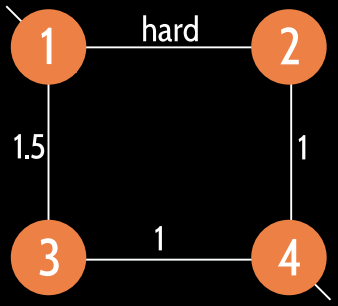

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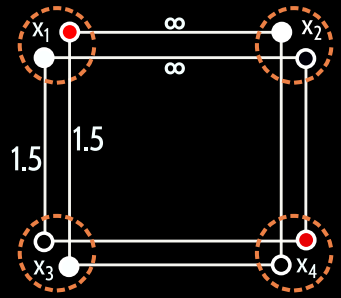


Min-CUT on 4 variables

```
{
   "problem" :{"name": "MinCut", "mustbe": "<100.0"},
     variables: {"x1": ["l"], "x2": ["l","r"],
                 "x3": ["l","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 $\{1, \cdots, 9\}$
- 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

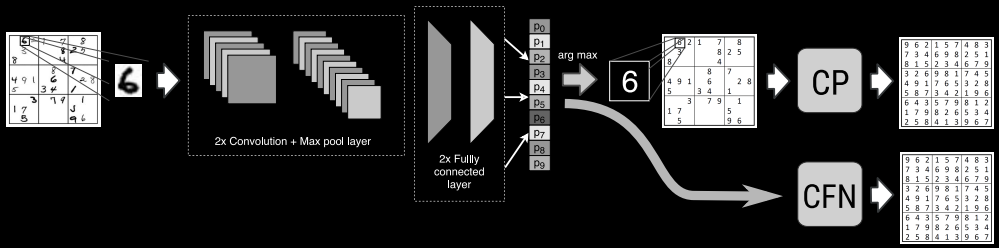
Let's have a look at the pytoulbar2 code.

```
myCFN = pytoulbar2.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

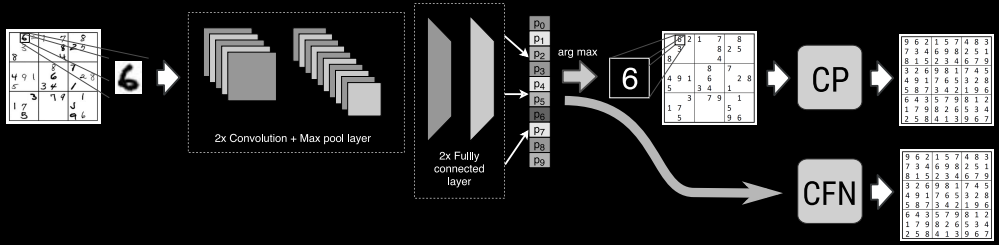
Thanks to Tias Gun for the picture above

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.

Numbers: interfacing with DL



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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 approach[1]

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

Tight links with (I)LP

Let's look at the primal connection

[1] Maxime 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.

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- 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

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

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

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

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

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

Presentation Outline

Systematic tree search — Time $O(d^n)$, linear space

- If all $|D^X| = 1$ obvious minimum — update k to $\Phi_{\mathcal{M}}(\boldsymbol{v})$
- Else choose $X \in \boldsymbol{V}$ 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

Optimization — Branch and Bound [LW66]

If the $\underbrace{\text{local lower bound}}_{\varphi_\varnothing}$ reaches the $\underbrace{\text{global upper bound}}_{k}$ Prune!

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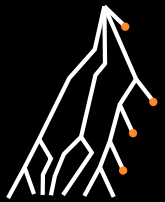
Depth First (CP) or Best First (ILP)?

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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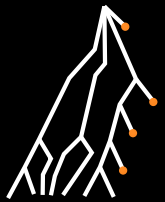

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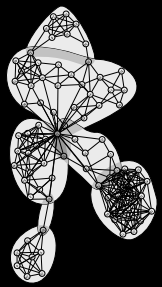

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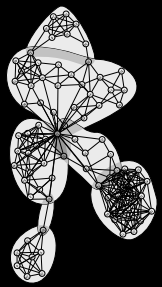

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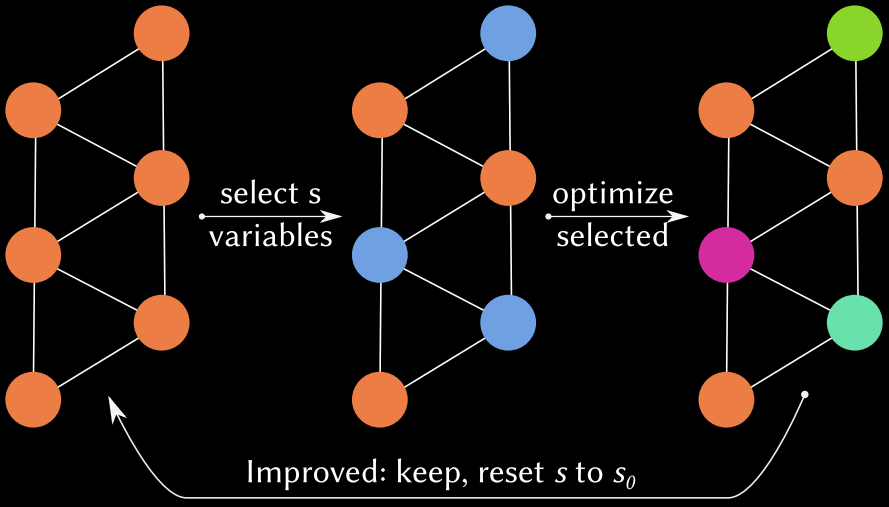
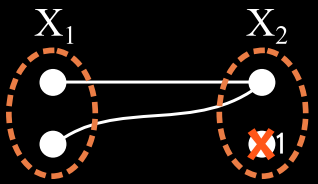
Also local search of course (VNS here)



Presentation Outline

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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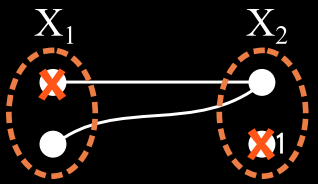

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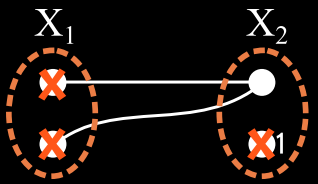

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One cannot add functions to the CFN: loss of equivalence, meaningless result

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

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- Subtract it from its source using $-^k$

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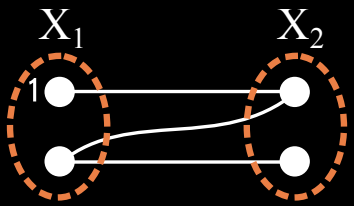
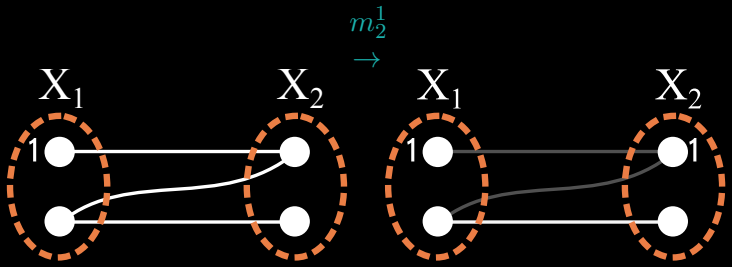


(Loss of) properties

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

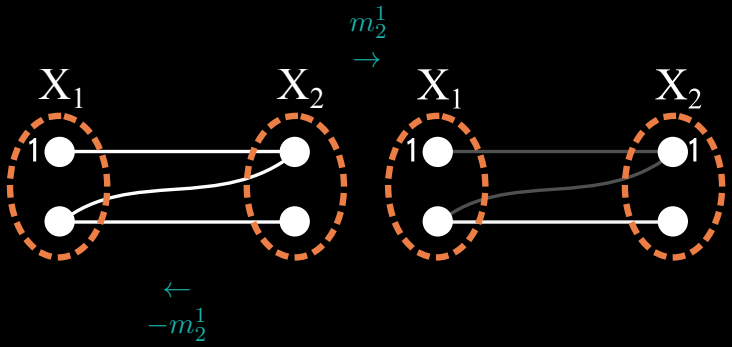
Example with $k > 1$



(Loss of) properties

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

Example with $k > 1$



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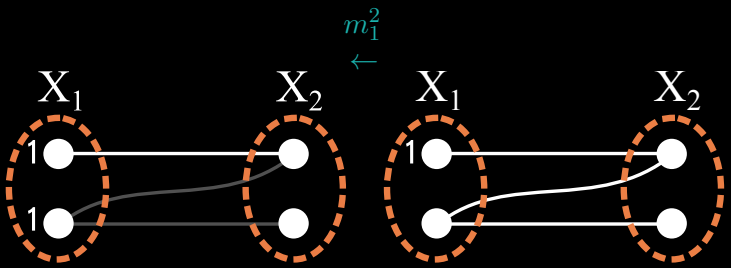

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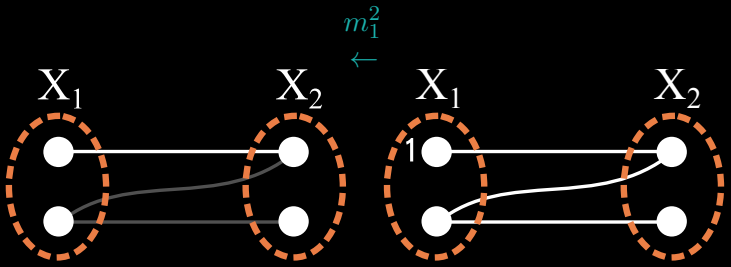

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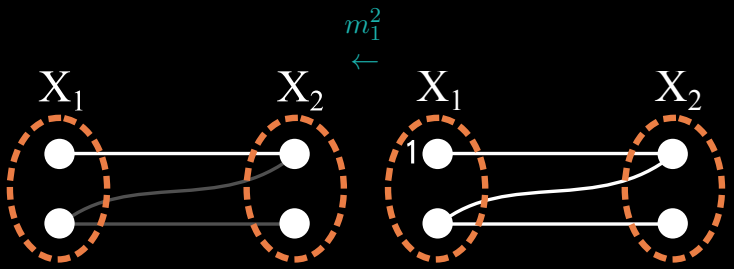

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Many way to avoid loops (enforce fixpoint existence)

ANITI INRAE

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

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- Polynomial time, $O(ed)$ space (Generalized ACs)
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- Stronger bounds than AC in COP [LL12]

Set of rational EPTs — OSAC [Sch76; Coo07; Wer07; Coo+10]

Maximizing $\varphi_\varnothing$ 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 $\varphi_\varnothing$
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

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

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

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

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The power of VAC and OSAC

ANITI INRAE

Problems solved [Coo+10; KZ17]

- Tree-structured problems
- Permutated 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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Presentation Outline

Additional algorithmic ingredients

- Value ordering (for free): existential or virtual supports
- Variable ordering: weighted degree [Bou+04], last conflict [Lec+09], VAC-based [TGK20]
- (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

Presentation Outline

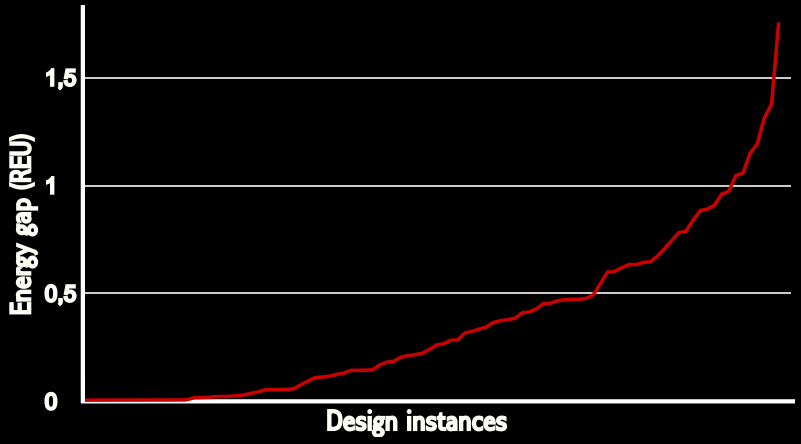
VAC vs. LP on Protein design problems

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)

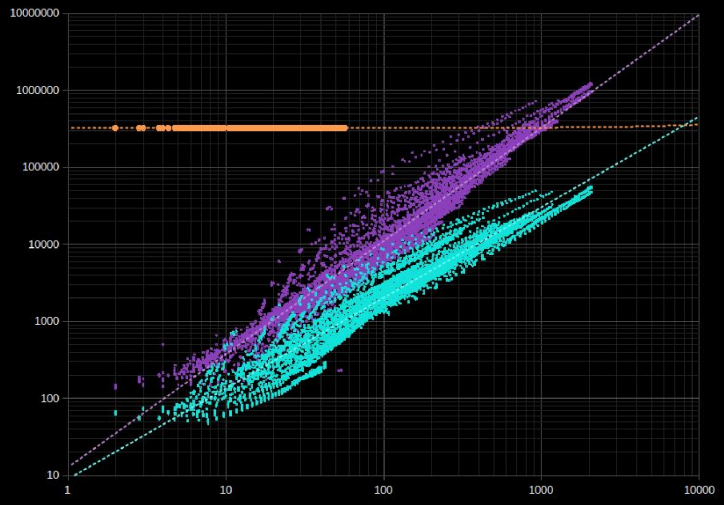
```
loading CFN file: 3e4h.wcsp
Lb after VAC: 150023297067
Preprocessing time: 9.13 seconds.
Optimum: 150023297067 in 129 backtracks, 129 nodes and 9.38 seconds.
```



Optimality gap of the Simulated annealing solution as problems get harder

[2] David 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.

Quantum computing (DWave),Toulbar2 & SA [Mul+19]



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 Designers[3]

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]

[3] Mark A Hallen and Bruce R Donald. "Protein design by provable algorithms". In: *Communications of the ACM* 62.10 (2019), pp. 76–84.

[4] Stefan Haller, Paul Swoboda, and Bogdan Savchynskyy. "Exact MAP-Inference by Confining Combinatorial Search with LP Relaxation". In: *Thirty-Second AAAI Conference on Artificial Intelligence*. 2018.

On Toulbar2 performances

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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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Pytoulbar2 code

```
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

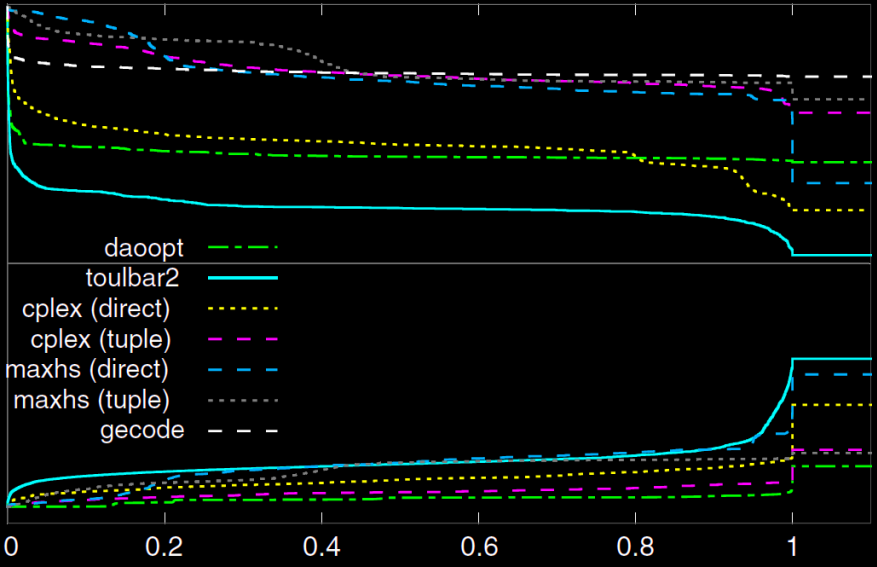
Je n'ai pas vraiment trouvé de cas [...] défavorable pour toulbar2.

3026 instances of various origins genoweb.toulouse.inra.fr/~degivry/evalgm

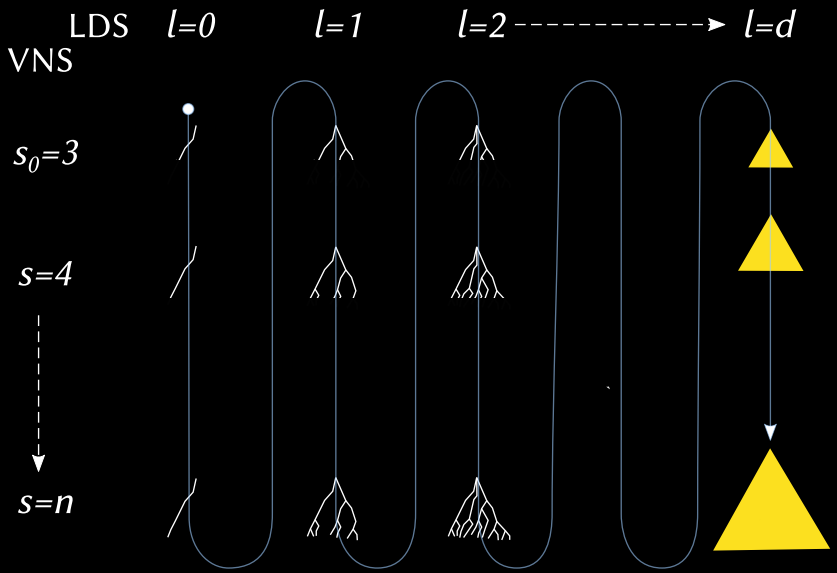
- MRF: Probabilistic Inference Challenge 2011
- CVPR: Computer Vision & Pattern Recognition OpenGM2
- CFN: Cost Function Library (CELAR, SPOT5, bioinformatics)
- MaxCSP: MaxCSP 2008 competition
- WPMS: Weighted Partial MaxSAT evaluation 2013
- CP: MiniZinc challenge 2012/13 (decomposable)

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

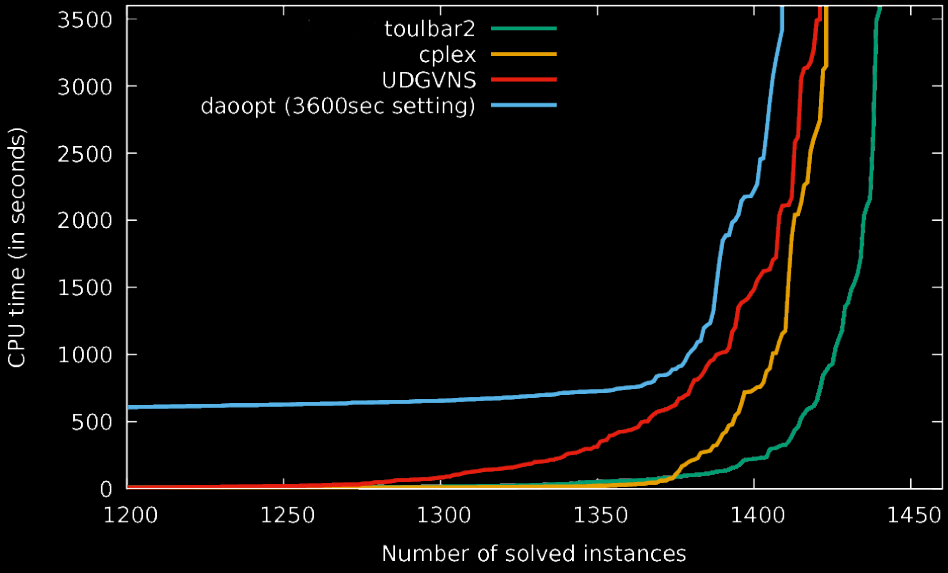
HBFS - Normalized lb and ub profiles (hard problems) [Hur+16]



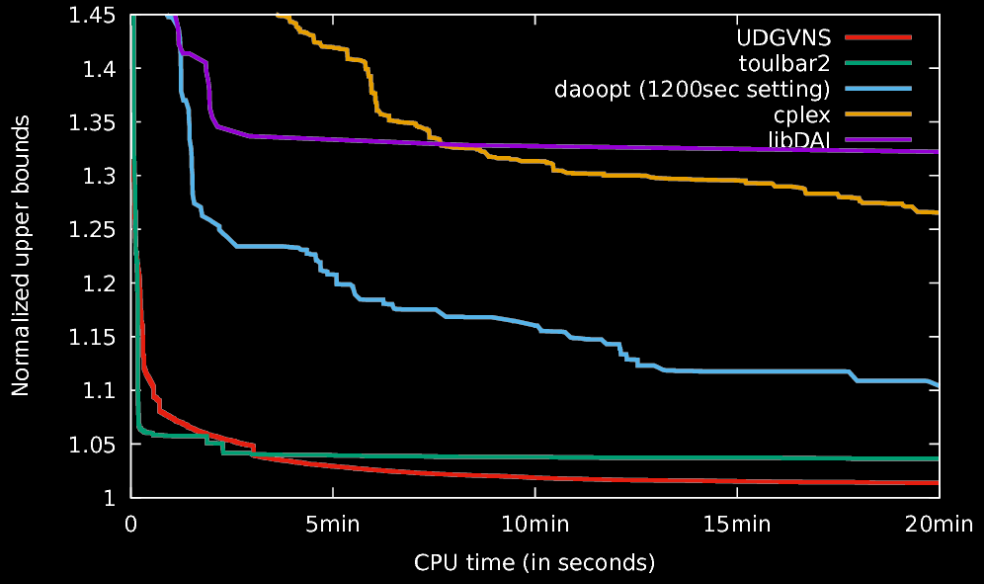
Unified Decomposition Guided VNS [Oua+20; Oua+17]



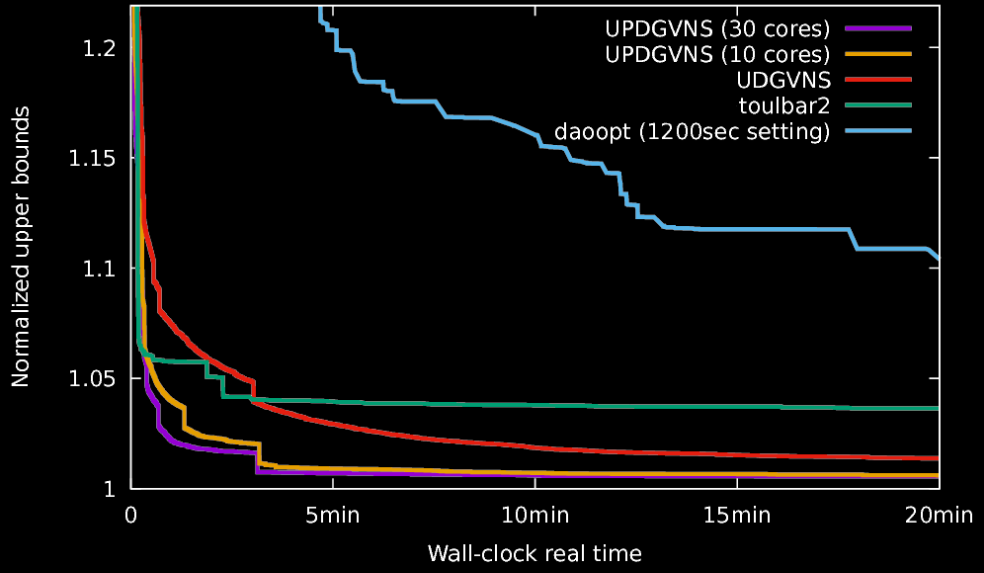
UDGVNS - Number of solved problems [Oua+17]



UDGVNS - Upper bound profiles[OUA+17]



UPDGVNS - Upper bound profiles[OUA+20]



Presentation Outline

Learning from historical solutions [BGS20]

Definition (Learning a pairwise CFN from high quality solutions)

Given:

- a set of variables $\boldsymbol{V}$,
- 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

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 $\boldsymbol{V}$
- Interpret costs as energies ($\propto -\log$(probabilities))
- Maximize the probability of observing the samples in E

Maximum loglikelihood $\mathcal{M}$ on $\mathcal{M}_\ell$

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

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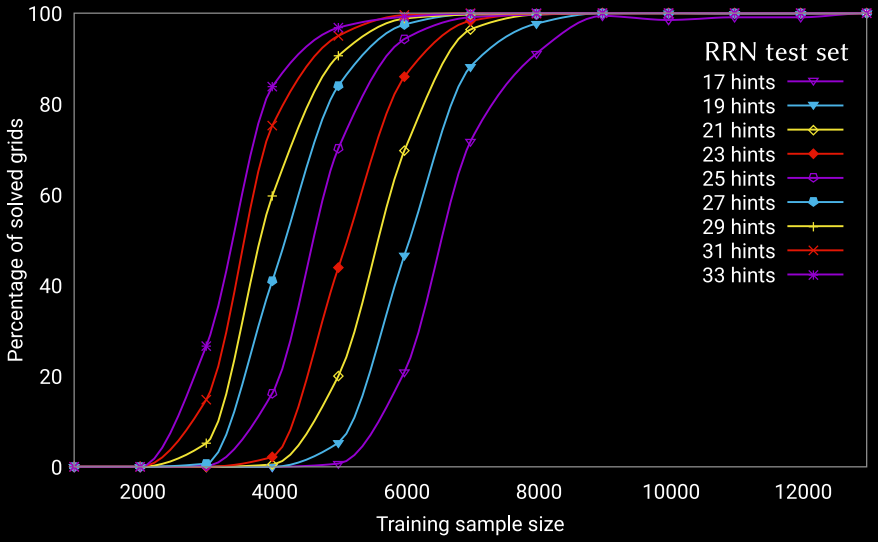
Algorithms and data-sets

- PE-MRF [Par+17] with L1-norm Regularization
- Validation set from the SAT-Net paper[5] (36.2 hints)
- Validation set from the RRN paper[6] with 17-34 hints.

[5] Po-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.

[6] Rasmus 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



RRN: 99.6%
(50,000 samples
per type given)

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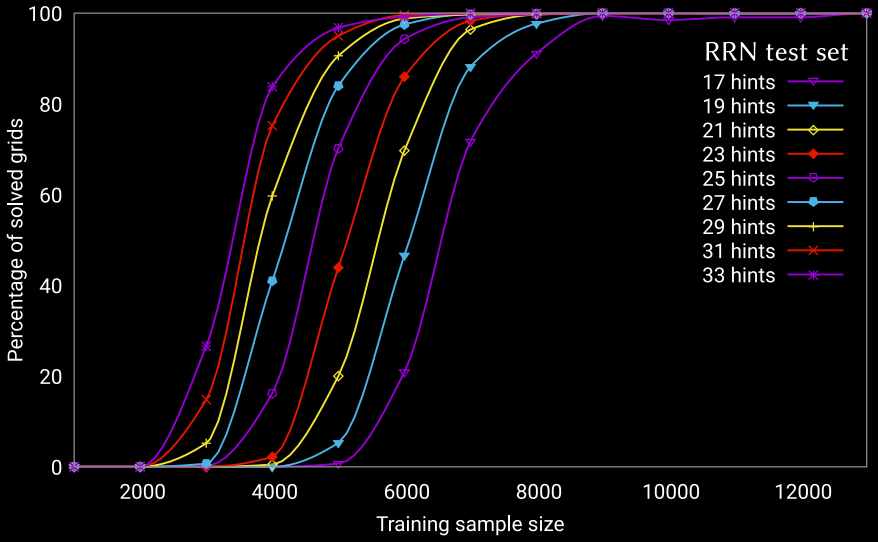

RRN: 96.6%
180,000 samples
(scopes given)

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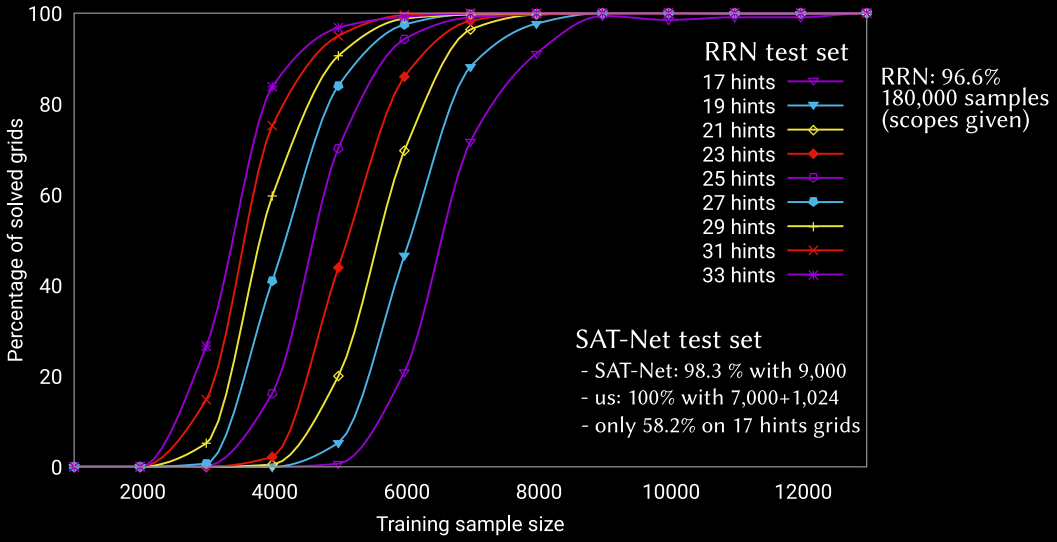

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Learning from images by connecting with PyTorch as before

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 paper[7]

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

[7] Céline 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.

A conclusion

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

A lot remains to be done

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

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C. Viricel (PhD)
A. Ouali (GREYC)
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M. Fontaine (GREYC, Caen)
C. Terrioux (LSIS)
Y. Lebbah (GREYC)
Mario (CU. Hong-Kong)
B. Hurley (Insight)
...

Questions?

[All+14] David Allouche et al. “Computational protein design as an optimization problem”. In: *Artificial Intelligence* 212 (2014), pp. 59–79.

[All+15] David Allouche et al. “Anytime Hybrid Best-First Search with Tree Decomposition for Weighted CSP”. In: *Principles and Practice of Constraint Programming*. Springer. 2015, pp. 12–29.

[All+16] David Allouche et al. “Tractability-preserving transformations of global cost functions”. In: *Artificial Intelligence* 238 (2016), pp. 166–189.

[BdS20] Céline 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.

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