## Constraint \& Cost Function Networks: <br> Feasibility, optimization and learning <br> JFPC'2021

## T. Schiex (AND plenty of colleagues)

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June 22, 2021

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

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


## Joint truth function



## The Constraint Satisfaction Problem (NP-complete)

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\Phi_{\mathcal{M}}=\bigwedge_{\varphi_{S} \in \Phi} \varphi_{S}
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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 $\varphi_{S}$

- 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)

$$
\left[\begin{array}{lll}
f & t & t \\
t & f & t \\
t & t & f
\end{array}\right]
$$

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

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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 $V$
- a set $\Phi$ of $e$ integer cost functions
- Each $\varphi_{S} \in \Phi$ is a numerical function bounded by $k$ (finite or infinite)

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

$$
\Phi_{\mathcal{M}}=\sum_{\varphi_{S} \in \Phi}^{k} \varphi_{\boldsymbol{S}}
$$

## The Weighted Constraint Satisfaction Problem (decision NP-complete)

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


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Tables (or tensors) for $\varphi_{S}$

- A multidimensional table with a number for every tuple in $D^{S}$


## Global functions

- Names for snecific (useful) functions

Soft difference (3 values)

$$
\left[\begin{array}{lll}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{array}\right]
$$

## A useful one

KNAPSACKS

Tables (or tensors) for $\varphi_{S}$
A multidimensional table with a number for every tuple in $D^{S}$

Global functions

- Names for specific (useful) functions


## Soft difference (3 values)



A useful one<br>KNAPSACK $_{S}$

## 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



- shifting: negative numbers and maximization ....................................................

Extra assumptions inside the solver

- CFNs have all unary functions $\varphi_{i}, X_{i} \in V$
- 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 $e=(i, j) \in E: \varphi_{i j}=w(i, j) \times \mathbb{1}\left[x_{i} \neq x_{j}\right]$


## A simple graph

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


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## 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 $X_{i j}$ 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

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
Add 'LeNet output tensor (negated) as a cost function $\left(\min \sum-\log \right) \equiv(\max$ I) probabilities


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The Numbers way

1. Add LeNet output tensor (negated) as a cost function
2. $\left(\min \sum-\log \right) \equiv(\max \Pi)$ probabilities >99\% acc.
```
myCFN = pytoulbar2.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 approach ${ }^{1}$

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


## Tight links with (I)LP

Let's look at the primal connection

[^0]
## CFN compared to a COP approach ${ }^{1}$

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■ CFN (toulbar2) + pairwise differences .............................................................0.05"

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- $99.6 \%$ of all problems are solved backtrack-free by toulbar2
- CFN bounds way tighter than COP bounds [LL12]


## Tight links with (I)LP

Let's look at the primal connection

[^3]The "local polytope" [Sch76; Kos99; Wer07]

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

$$
\begin{array}{lr}
\sum_{a \in D^{i}} x_{i a}=1 & \forall i \in\{1, \ldots, n\} \\
\sum_{b \in D^{j}} y_{i a j b}=x_{i a} & \forall \varphi_{i j} \in \Phi, \forall a \in D^{i} \\
\sum_{a \in D^{i}} y_{i a j b}=x_{j b} & \forall \varphi_{i j} \in \Phi, \forall b \in D^{j} \\
x_{i a} \in\{0,1\} & \forall i \in\{1, \ldots, n\}
\end{array}
$$

$n d+e d^{2}$ variables, $n+2 e d$ 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

- 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 set $X=u$
2. one where $u$ is removed from $D^{X}$

- Return the minimum
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If the local lower bound reaches the global upper bound

## 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



## Nice properties

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


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Else: forget, set $s$ to $s+1$

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## Filtering by Arc Consistency (support)

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


## Properties

- Combine $\varphi_{i j}$ and $\varphi_{j}$
- Project on $X$
- Combine with $\varphi_{i}$
- Uninue fixnoint (monotonic), polynomial time


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- Combine with $\varphi_{i}$
- Unique fixpoint (monotonic), polynomial time

Obvious issue
One cannot add functions to the CFN: loss of equivalence, meaningless result
$\square$
Equivalence Preserving Transformations with

- Add the projection to $\varphi_{i}$ with $+^{k}$
- Subtract it from its source using - ${ }^{k}$


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One cannot add functions to 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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$m_{1}^{2}$


$$
\begin{aligned}
& \Downarrow \\
& \varphi_{\varnothing}=1
\end{aligned}
$$

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## The many "soft ACs"

One paper to read: [Coo+10]

- NC+AC+DAC (FDAC): binary \& unary (+ direction)[Schoo; Laro2; 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

## Supports provide value ordering heuristics

- EAC: $\varphi_{i}^{\prime}(u)=0$ 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]

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

- Proper extension of classical NC/DAC or AC respectively
- Polynomial time, $O(e d)$ space (Generalized ACs)
- Incremental, strengthens $\varphi_{\varnothing}$ $(\mathrm{NC} \leq \mathrm{AC} \leq \mathrm{FDAC} \leq \mathrm{EDAC} \leq \mathrm{VAC})$
- Stronger bounds than AC in COP [LL12]

Set of rational EPTs
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 $\varphi_{i}$ 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

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

Problems solved [Coo+10; KZ17]

- Tree-structured problems
- Permutated submodular problems


## OSAC empirically too expensive compared to VAC

- CFN Arc consistencies nrovide fact annrovimate I P hounds
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## CFN Local Consistencies

Enhance $C P$ with fast incremental approximate Linear Programming dual bounds

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## 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 [Laroo]

■ 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

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## 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
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

[^5]
## Quantum computing (DWave),Toulbar2 er SA [Mul+19]



DWave approximations

## 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 CPI EX wariants in all our testc"

[^6]
## 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

[^7]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

Dresented in [Den 17. Der:-101 dominates MILP and MIQCP

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.
def generate_model(path):
$\mathrm{m}=$ 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.

- 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 | 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 |




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

NNITI
NRAO



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

## 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

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 $\left|D^{i}\right| \times\left|D^{j}\right|$ costs in $\mathbb{R}$ (differentiability)
- 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 ( $\propto-\log$ (probabilities))
- Maximize the probability of observing the samples in $E$


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



## Maximum likelihood estimation

- $E$ a set of i.i.d. assignments of $V$
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## Maximum loglikelihood $\mathcal{M}$ on $\mathcal{M}_{\ell}$

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

## Learning how to solve the Sudoku

## 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.

[^8]



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 <br> - SAT-Net (9,000 samptes): <br> - Toulbar $2+$ PE-MRF $(8,000+1,024$ samples $):$

## 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):

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)).

[^9]
## 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)
- ...

```
And to all CFN/toulbar2 contributors
```

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B. Hurley (Insight)

## Questions?

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[^1]:    ${ }^{1}$ 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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[^4]:    NC provides reduced cost-based pruning (back-propagation)

    $$
    \text { If }\left(\rho_{x} \not{ }^{k} \omega_{i}(u)\right)=k \text { NC deletes } u .
    $$

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