Graphical Models

Logic, costs, & probabilities

Nesy-Montreal

T. Schiex

Université Fédérale de Toulouse, ANITI, INRAE MIAT, Toulouse, France

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Graphical models [16, 30, 20, 37]

The definition of a multivariate function as the *combination* of *simple* functions.

- Constraint networks, SAT (CNF), CP: boolean, feasibility
- Cost Function Networks, Max-SAT, COP: cost and feasibility
- Markov Random Fields, Bayesian Nets: probabilities (normalization)
- Algebraic frameworks (Valued/monoïds [32], Semi-Ring [36, 8, 24]),…

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

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

Joint truth function

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

The Constraint Satisfaction Problem (NP-complete)

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

GMs for feasibility (combination operator)

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Languages for domains and constraints

- Constraint Networks: Boolean tables (tensors) for domains and constraints
- SAT/CNF: Boolean variables and clauses
- Constraint Programming: interval domains, specialized constraints

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)

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

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Beyond dense tensors

- Clauses: forbids one cell of a (sparse) tensor
- Names for specific (useful) constraints

GMs for feasibility (language): CN, SAT, CP

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Most famous

AllDifferent$s$

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Languages for domains and constraints

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- Constraint Programming: interval domains, specialized constraints

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?

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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 $\varphi_{\boldsymbol{S}} \in \Phi$ is a numerical function bounded by k (finite or infinite)

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

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

The Weighted Constraint Satisfaction Problem (decision NP-complete)

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

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- Weighted clauses: a cost for a cell in a (sparse) tensor
- Names for specific (useful) functions

Soft difference (3 values)

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

Example

$\textsc{WeightedRegular}_{\mathcal{A},S}$

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$\textsc{WeightedRegular}_{\mathcal{A},S}$

COP uses a suitably constrained variable to represent a cost.

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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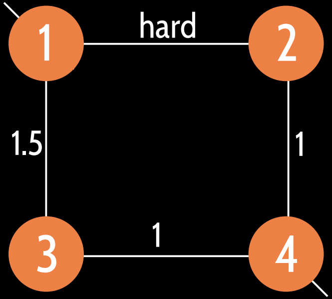


Min-CUT on 4 variables

```
import pytoulbar2
myCFN = pytoulbar2.CFN(100,1)   # k/ub, resolution
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

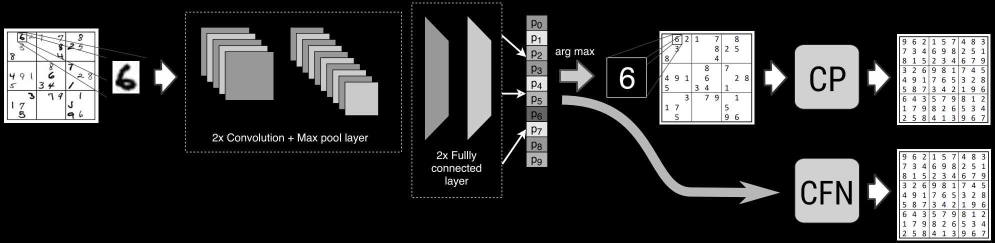
Let's have a look at the pytoulbar2 code.

```
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

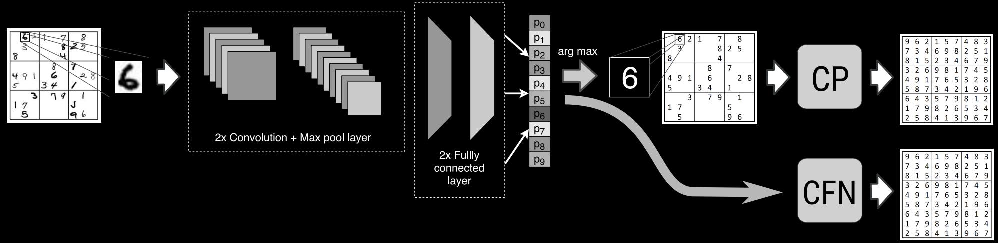
Thanks to Tias Gun for the picture above

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 logits (negated) as a cost function
2. $(\min \sum -\log) \equiv (\max \prod)$ probabilities . . . . >99% acc.

Numbers: interfacing with ML/DL



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myCFN = pytoulbar2.CFN(1000000000,6)

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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[1,2]

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

[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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CFN compared to a COP approach[1,2]

- COP (OR-Tools) + global All-Different . . . . 0.79"
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- COP (OR-Tools) + global All-Different . . . . 0.79"
- CFN (toulbar2) + pairwise differences . . . . .0.05"
- 99.6% of all problems are solved backtrack-free by toulbar2
- CFN bounds way tighter than COP bounds [25]

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Combination and normalisation

- log-linear models (or multiplication)

$$P(t) \propto \exp(-\Phi(t))$$

- optimisation and counting (marginals)
- Normalization is #P-hard.
- High probabilities for good solutions

Markov Random Fields, Bayesian nets, Factor Graphs, Ising/Potts models [19]

- log-linear MRFs $\approx$ CFNs (cost = energy). Image/signal processing.
- Bayes-nets use a DAG product-rule decomposition ($P(A, B) = P(A|B).P(B)$)
- Higher-order factors $\approx$ global constraints

Many theorems and algorithms assume $P(t) > 0$.

Pairwise models [1]

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

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

$$x_{ia} \in \{0,1\} \qquad \forall i \in \{1, \ldots, n\}$$

nd variables, n constraints: concise but challenging

The universal "local polytope" [34, 22, 39, 38] (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

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

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

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

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

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

As an NP-hard discrete optimization framework

Discrete Graphical Models

- Are polynomials in their decision variables (OHE)
- Criterion linear in the finite parameters (costs)
- Criterion and constraints are homogeneous, but
- Additive $(a + a = 2a)$ and idempotent $(a + a = a)$ respectively

Non serial Dynamic Programming [3, 2, 4]

- Tree-decompositions [33] and compilation: OBDD, d-DNNF, SDD, ADD [17] vs. Lauritzen/Shafer hypergraph message passing [35, 24], ...
- Exact, operator flexible (semi-ring), differentiable, but space and time exponential

Local reasoning

- (soft) local consistencies/UP/max-resolution [31, 23] vs. (convergent) belief propagation [39, 21] (LP dual)
- Solves tree-structured/(submodular) min-max closed problems
- Efficient, bounds (convergent), heuristics (CP-BP [13]).

Optimisation/decoding and counting/inference

Tree search

- Backtrack, Branch and Bound, …(optimisation, counting), hashing [14]
- Exact, exponential time.

Random search

- Local search (optimisation) vs. MCMC sampling (counting)
- Asymptotic properties, arbitrary time and quality

Relaxations

- LP [39] and convex SDP [38, 18] (Max2SAT, Pairwise additive GMs)
- Poly. time, differentiable, but approximate.

Deterministic models

From a set of (optimal) solutions (or non-solutions)

- Constraint acquisition [7]
- Preference elicitation [11]
- related to classical inverse optimisation [15] (LP, convex, conic, ILP)

Stochastic models

From a fair sample

- Maximum log-likelihood (Z, CRF loss)
- Structured Perceptron/Hinge losses,...
- Fenchel-Young losses [9, 27, 5, 29] (regularization)
- Mean field/variational [38]
- Approximate [37, 28], Pseudo likelihoods [6]

Thank you all for your attention!

And to all CFN/toulbar2 contributors

S. de Givry (INRAE)	G. Katsirelos (INRAE)	M. Zytnicki (PhD, INRAE)
D. Allouche (INRAE)	M. Ruffini (PhD)	H. Nguyen (PhD)
M. Cooper (IRIT, Toulouse)	J. Larrosa (UPC, Spain)	F. Heras (UPC, Spain)
M. Sanchez (PostDoc)	E. Rollon (UPC, Spain)	P. Meseguer (CSIC, Spain)
G. Verfaillie (ONERA, ret.)	JH. Lee (CU. Hong Kong)	C. Bessiere (LIMM, Montpellier)
JP. Métivier (GREYC, Caen)	S. Loudni (GREYC, Caen)	M. Fontaine (GREYC, Caen)
D. Simoncini (PostDoc, UT1)	C. Viricel (PhD)	C. Terrioux (LSIS)
P. Jégou (LSIS)	A. Ouali (GREYC)	Y. Lebbah (GREYC)
L. Loukil (GREYC)	P. Boizumault (GREYC)	Mario (CU. Hong-Kong)
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Questions?

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