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Toulbar2: optimizing discrete multivariate models

Graphical models & Constraint programming

T. Schiex & S. de Givry

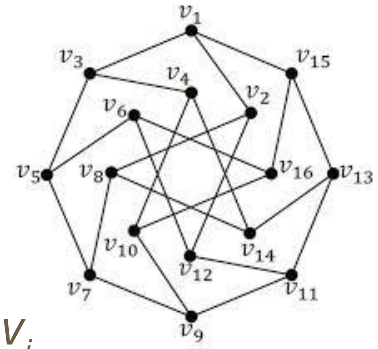
github.com/toulbar2/toulbar2 pip3 install pytoulbar2 toulbar2.github.io/toulbar2

Modeling: Cost Function Networks (CFN)

- Discrete variables: $X_1,...X_n$
- Joint function on these: $E(X_1,...X_n) = -\log(P(X_1,...,X_n)) + cte$
- E is "infinite-valued" (E = ∞ ≍ false ≍ zero probability) 64 bits
- Described as the sum of "elementary" functions
  - Cost tables (tensors, space exponential in the number of involved variables)
  - Predefined global functions: *AllDiff*$(X_1,...X_m)$, *Regular*$(A, X_1,.., X_m)$, *Knapsack*$(A,c,X_1,.., X_n)$...
- Many representable frameworks (many file formats):
  - SAT, weighted MaxSAT, (quadratic) Pseudo-Boolean & 01LP, QUBO, CP/COP (XCSP3)
  - Hidden Markov Models, Markov Random Fields, Bayesian nets (UAI)

Graphs *(V,E)* & colors *(k)*

- One variable X_i per vertex $i \in V$
- Domains = possible colors
- *k*-coloring : for each $(i,j) \in E$, $f_{ij} \propto$ *eye(k)*
- min-*cost* k-coloring : adding f_i
- max-k-coloring: relaxing f_{ij}
- Cost from f_{ij} and f_i are added
- possible separation of costs (Pareto)



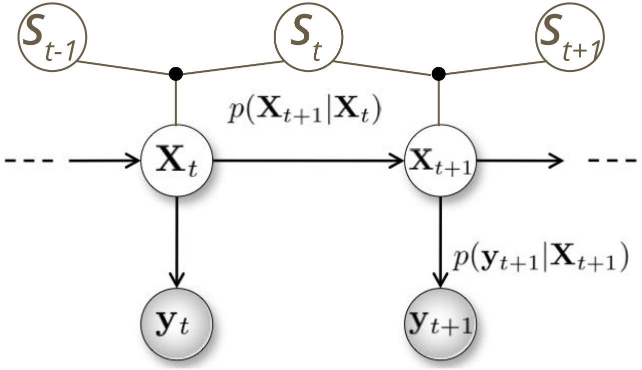
$$\begin{array}{cc} & v_j \\ v_i & \begin{bmatrix} \infty & 0 & 0 \\ 0 & \infty & 0 \\ 0 & 0 & \infty \end{bmatrix} \end{array} \qquad \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

0	1	2

```
infinite = 1000000
cfn = pytoulbar2.CFN(infinite)
for i in V: cfn.AddVariable('X'+str(i),range(k))
for (i,j) in E: cfn.AddFunction(['X'+str(i),'X'+str(j)],infinite*np.eye(k).flatten())
cfn.Solve()
```

Hidden Markov Model

- Variables X_t and Y_t with their domains
- Functions $f(X_t, Y_t) = -log(p(Y_t|X_t))$ and $f(X_{t+1},X_t) = -log(p(X_{t+1}|X_t))$
- Treewidth = 1 (acyclic)... dynamic programming
- The succession of hidden states belongs to a regular language (automata)
- $Regular(A,X_1,...,X_n)$ decomposable in tables $A(S_i,X_i,S_{i+1})$



Various algorithms for 3 main queries

1. Find $(x_1,\dots x_n)$ minimizing $E(x_1,\dots,x_n)$ decision NP-complete
   a. optimality proof by default (logical reasoning & *reductio ad absurdum*)
   b. anytime, with shrinking optimality gap (predefined or on the fly)
   c. branch & bound with dedicated bounds (generalized CP/SAT inference, cvgt Message Passing)
   d. depth-first or hybrid best/depth first search (default)
   e. can exploit the problem structure (treewidth)
   f. exhaustive local search (VNS-LDS), better solutions faster but...
   g. C++ multi-core (MPI) implementation
   h. Python API (`pip3 install pytoulbar2`) - Linux/MacOS (Windows soon!)
2. Counting (solutions, partition function) #P-complete
   a. exact algorithms (very expensive except for structured problems)
   b. approximation with deterministic guarantee (same, but tunable)
3. Bi-objective optimization (Pareto front) https://forgemia.inra.fr/samuel.buchet/tb2_twophase

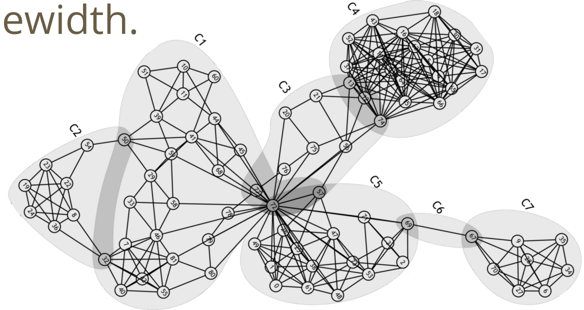
Winner of Max-CSP/COP (CPAI08, XCSP3 2022, 2023, 2024) and graphical models (UAI 2008, 2010, 2014, 2022 MAP task) challenges.

Max-Cut vs Min-Cut, MRF-based image segmentation

- Graph (V,E) with two colors (vertices partition, symmetry)
- MaxCut: for every $e_{ij} \in E$, $f_{ij} = -\mathbb{1}[X_i \neq X_j]$ (minimization)
  - f_{ij} is supermodular: NP-hard
- MinCut: for every $e_{ij} \in E$, $f_{ij} = \mathbb{1}[X_i \neq X_j]$ (minimization)
  - fij is submodular: polytime (one bound, VAC, gives this polytime behavior)
- Image segmentation: Hidden Markov Random Field, still submodular
  - use dedicated implementations (V. Kolmogorov) for pure segmentation
  - used as the last “layer” of neural architectures for detailed semantic segmentation.

Radio Link Frequency Assignment (CELAR)

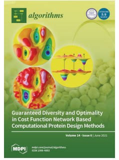
- Generalization of *k*-coloring
- Set of radio links with available frequencies (variables)
- “Nearby” links must use sufficiently different frequencies $f_{ij} = \infty \times \mathbb{1}|X_i\text{-}X_j < k|$
- Extra technological constraints (constant emission/reception frequency shift)
- Criteria:
  - minimize the number of frequencies used (*N-values* global constraint)
  - minimize the number of links subject to interference (replace ∞ by dedicated costs)
- Spatial interactions => smaller treewidth.



Weaknesses & Strengths

- Not good for very large domains (time, scheduling)
- Not so good for random problems
- Optimization>feasibility (use SAT/ILP/CP if natural)

- Loves problem with a majority of functions over few (<=3) variables
- Useful when ‘small’ treewidth, or submodularity is present
- Unexpected efficiency on physics-based Computational Protein Design



Guaranteed Discrete Energy Optimization on Large Protein Design Problems

David Simoncini[†], David Allouche[†], Simon de Givry[†], Céline Delmas[†], Sophie Barbe[‡§⊥], and Thomas Schiex[*†]

JCTC Journal of Chemical Theory and Computation

Learning models from solutions (self-supervised, stochastic interpretation)

- From a set of ‘good’ solutions
  - Approximate log-likelihood with L1/L2 regularisation (sparsistent, sufficient statistics)
  - Relies on convex optimisation (ADMM)
  - CFN-learn numpy-based package, separate from toulbar2.

  Learn customer preferences from configurations (Renault)
  Learn how to play Sudoku (9,000 solved grids)

  https://github.com/toulbar2/CFN-learn

- From a set of good solutions with associated information (~~supervision~~):
  - Deep learning based (in: informations, out: a CFN)
  - Emmental-PLL loss (improves Besag consistent pseudo-loglikelihood - IJCAI’23)
  - Emmental-PLL torch-based Package, separate from toulbar2 - limitations

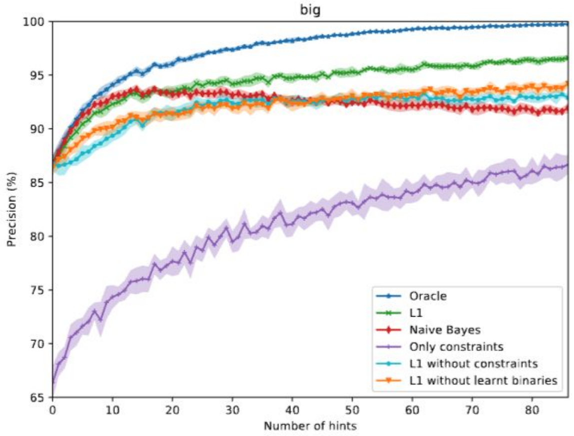
  Learn customer preferences from configurations (Renault) given age, SCP, gender
  Learn how to play Sudoku from the grid geometry (200 solved grids, image input)

  https://forgemia.inra.fr/marianne.defresne/emmental-pll

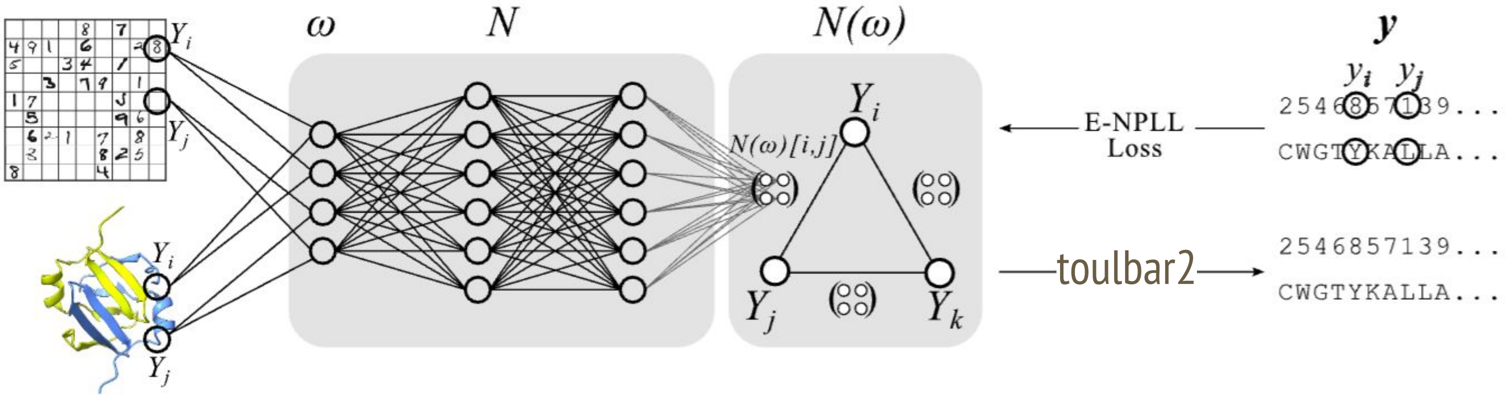
Learning preferences from configurations

Renault utility van with combinatorial options:

- 68 variables, 324 values, 332 constraints (12 vars), 8,337 configurations
- Up to 24, 566, 537, 954, 855, 758, 069, 760 different vehicles
- Learning user preferences from passed valid configurations
- 10-fold cross validation



Learning how to design proteins *(inverse folding)*



The learned representation of $p(y|\omega)$ can be constrained or biased arbitrarily w/o retraining.

Learning how to design proteins

Self-assembling complex

- Symmetry
- Specific interactions

Ancestral protein

- Symmetry
- Limited chemical variety

Nanobodies

- DDPM (loop generation)
- High affinity
- High specificity