Graphical Models – Queries, complexity, algorithms and applications

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Informally

A description of a multivariate function as the combination of a set of simple functions.

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Propositional logic (CNF aka Conjunctive Normal Form)

A Boolean function of Boolean variables described as the conjunction of disjunction of literals.

What is a graphical model?

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Discrete Markov Random Fields

A non negative function of discrete variables described as the product of non negative tensors.

Concisely describing complex systems

- Concise: we use a set of *small* functions.
- Complex: the joint function results from the interaction of several small functions.

Example

A digital circuit	value of the output
A Sudoku grid	solution or not
A schedule or a time-table	feasibility, acceptability
A pedigree with genotypes	Mendel consistency, probability
A frequency assignment	interference amount
A 3D molecule	energy, stability

Ideally, we would like to

- Learn them: from a sample [Par+17; PPW18]
- Compute their value: given a variable assignment
- Compute simple statistics:
  - Minimum/Maximum: optimization
  - Average: counting
  - ...

Concise and Complex

Plenty of NP-hard problems.

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- Variables: $X, Y, Z, \ldots$, possibly indexed as X_i or just i.
- Domains: D_X for variable X, or D_i for variable X_i.
- Values: $\mathtt{a}, \mathtt{b}, \mathtt{c}, \mathtt{g}, \mathtt{r}, \mathtt{t}, \mathtt{1} \ldots$
- Unknown values: $u, v, w, x, y, z \ldots$.
- Sequence of variables: $\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{Z}, \ldots$
- Sequence of values: acgtgcatggagccacgtcaggta
- Unknown sequence of values: $\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}, \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z} \ldots$.
- Domain of a sequence of variables $\boldsymbol{X} : D_{\boldsymbol{X}}$ (Cartesian product of the domains).
- Assignment $\boldsymbol{u}_{\boldsymbol{X}}$: an element of $D_{\boldsymbol{X}}$. Defines an assignment for all the variables in $\boldsymbol{X}$.
- $\boldsymbol{u}_{\boldsymbol{X}}[\boldsymbol{Y}]$ (or $\boldsymbol{u}_{\boldsymbol{Y}}$): *projection* of $\boldsymbol{u}_{\boldsymbol{X}}$ on $\boldsymbol{Y} \subseteq \boldsymbol{X}$ (the sequence of values of $\boldsymbol{Y}$ in $\boldsymbol{u}_{\boldsymbol{X}}$).

A definition parameterized by B and $\bigoplus$

Definition (Graphical Model (GM))

A GM $\mathcal{M} = \langle \boldsymbol{V}, \Phi \rangle$ with co-domain B and combination operator $\oplus$ is defined by:

- a sequence of n variables $\boldsymbol{V}$, each with an associated finite domain of size less than d.
- a set Φ of e functions (or factors).
- Each function $\varphi_{\boldsymbol{S}} \in \Phi$ is a function from $D_{\boldsymbol{S}} \rightarrow B$. $\boldsymbol{S}$ is called the scope of the function and $|\boldsymbol{S}|$ its arity.

Definition (Joint function)

$\mathcal{M}$ defines a joint function:

$$\Phi_{\mathcal{M}}(\boldsymbol{v}) = \bigoplus_{\varphi_{\boldsymbol{S}} \in \Phi} \varphi_{\boldsymbol{S}}(\boldsymbol{v}[\boldsymbol{S}])$$

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B

- B is assumed to be totally ordered by $\prec$.
- With a minimum element $\mathbf{0}$ and a maximum element denoted as $\top$.

$\bigoplus$

- Associative, commutative, monotonic. $(\alpha \succeq \beta \Rightarrow (\alpha \oplus \gamma) \succeq (\beta \oplus \gamma))$
- $\mathbf{0}$ as an identity. $(\alpha \oplus \mathbf{0} = \alpha)$
- $\top$ as an absorbing element. $(\alpha \oplus \top = \top)$

Optional

- Idempotency. $(\alpha \oplus \alpha = \alpha)$
- Fairness. $(\forall \beta \preccurlyeq \alpha, \exists \gamma \text{ s.t. } (\beta \oplus \gamma) = \alpha)$
- Denoted as $\gamma = (\alpha \ominus \beta)$ $(\beta \oplus (\alpha \ominus \beta) = \alpha)$

Structure (GM)	B	$a \oplus b$	$\prec$	$\mathbf{0}$	$\top$	Idemp.	$a \ominus b$
Boolean	$\{t, f\}$	$a \wedge b$	$t < f$	t	f	yes	a
Possibilistic	$[0, 1]$	$\max(a, b)$	$<$	0	1	yes	$\max(a, b)$
Additive	$\bar{\mathbb{N}}$	$a + b$	$<$	0	$+\infty$	no	$a - b$
Weighted	$\{0,1,\ldots,k\}$	$\min(k, a+b)$	$<$	0	k	no	$(a=k\ ?\ k\ :\ a-b)$
Probabilistic	$[0, 1]$	$a \times b$	$>$	1	0	no	a/b

Fair countable structures exhaustively analyzed [CS04; Coo05]

- Stack of additive/weighted structures
- Interacting as idempotent structures

How are functions $\varphi_{\boldsymbol{S}} \in \Phi$ represented?

- Default: as tensors over B. (multidimensional tables)
- Boolean vars: (weighted) clauses. (disjunction of literals: variables or their negation)
- Using a specific language, subset of all tensors or clauses or dedicated (All-Different).

This influences complexities

- We assume a constant time $\oplus$ and constant space representation of elements of B.
- We mostly use tensors (universal): $\varphi_{\boldsymbol{S}}$ represented in space $O(d^{|\boldsymbol{S}|})$.

A variety of well-studied frameworks

- Propositional Logic (PL): Boolean domains and co-domain, conjunction of clauses
- Constraint Networks (CN): Finite domains, Boolean co-domain, conjunction of tensors
- Cost Function Networks (CFN): Finite domains, numerical co-domain, sum of tensors.
- Markov Random Fields (MRF): Finite domains, $\mathbb{R}^+$ as co-domain, product of tensors.
- Bayesian Networks (BN): MRF + normalized functions and scopes following a DAG.
- Generalized Additive Independence [BG95], Weighted PL, QPBO [BH02], ILP…

Excluded

- Gaussian Graphical Models or Linear Programming.
- Totally ordered B excludes e.g. Ceteris Paribus networks (CP-nets [Dom+03])

Definition (Equivalence)

Two graphical models $\mathcal{M} = \langle \boldsymbol{V}, \Phi \rangle$ and $\mathcal{M}' = \langle \boldsymbol{V}, \Phi' \rangle$, with the same variables and valuation structure are equivalent iff they define the same joint function:

$$\forall \boldsymbol{v} \in D_{\boldsymbol{V}}, \Phi_{\mathcal{M}}(\boldsymbol{v}) = \Phi_{\mathcal{M}'}(\boldsymbol{v})$$

Definition (Relaxation)

Given two graphical models $\mathcal{M} = \langle \boldsymbol{V}, \Phi \rangle$ and $\mathcal{M}' = \langle \boldsymbol{V}, \Phi' \rangle$, with the same variables and valuation structure, $\mathcal{M}$ is a relaxation of $\mathcal{M}'$ iff

$$\forall \boldsymbol{v} \in D_{\boldsymbol{V}}, \Phi_{\mathcal{M}}(\boldsymbol{v}) \preccurlyeq \Phi_{\mathcal{M}'}(\boldsymbol{v})$$

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Definition ((Hyper)graph of $\mathcal{M} = \langle \boldsymbol{V}, \Phi \rangle$)

One vertex per variable, one (hyper)edge per scope $\boldsymbol{S}$ of function $\varphi_{\boldsymbol{S}} \in \Phi$.

Definition (Factor graph of $\mathcal{M} = \langle \boldsymbol{V}, \Phi \rangle$)

The bi-partite incidence graph of the hypergraph above. One vertex per variable or function, an edge connects the vertex $\varphi_{\boldsymbol{s}}$ to all variables in $\boldsymbol{S}$.

Definition (Primal/Moral graph of $\mathcal{M} = \langle \boldsymbol{V}, \Phi \rangle$)

The 2-section of its hypergraph.

Definition (Micro-structure graph of $\mathcal{M} = \langle \boldsymbol{V}, \Phi \rangle$)

Weighted n-partite graph with one vertex per value and a weighted hyper-edge on $\boldsymbol{s} \in D_{\boldsymbol{S}}$ for every $\varphi_{\boldsymbol{S}} \in \Phi$ and $\boldsymbol{s}$ such that $\varphi_{\boldsymbol{S}}(\boldsymbol{s}) \neq \boldsymbol{0}$.

CFN $\mathcal{M} = \langle V, \Phi \rangle$, parameterized by $k = \top$

$\mathcal{M}$ defines a non negative joint function $\Phi_{\mathcal{M}} = \min(\sum_{\varphi_S \in \Phi} \varphi_S, k)$

Flexible

- $k = 1$ same as Constraint Networks
- $k = \infty$ same as GAI, $-\log()$ transform of MRFs
- k finite k is a known upper bound
- $\varphi_\varnothing$ is a naive lower bound on the minimum cost

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Optimization queries

- SAT/PL: is the minimum of $\Phi_{\mathcal{M}} = t$?
- CSP/CN: is the minimum of $\Phi_{\mathcal{M}} = t$?
- WCSP/CFN: is the minimum of $\Phi_{\mathcal{M}} \prec \alpha$?
- MAP/MRF: is the minimum of $\Phi_{\mathcal{M}} \prec \alpha$?
- MPE/BN: is the minimum of $\Phi_{\mathcal{M}} \prec \alpha$?

Counting queries

- #-SAT/PL: how many assignments satisfy $\Phi_{\mathcal{M}} = t$?
- MAR/MRF: compute $Z = \sum(\Phi_{\mathcal{M}})$ or $P_{\mathcal{M}}(X = u)$ where $X \in \boldsymbol{V}$
- MAR/BN: compute $P_{\mathcal{M}}(X = u)$ where $X \in \boldsymbol{V}$

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Using $\bigotimes$ as a marginalization or elimination operator

$$\bigotimes_{v \in D_V} \left[\bigoplus_{\varphi_S \in \Phi} (\varphi_S(v[S])) \right]$$

$\otimes$ associative, commutative, distributive $\alpha \oplus (\beta \otimes \gamma) = (\alpha \oplus \beta) \otimes (\alpha \oplus \gamma)$

Axioms for dynamic programming

Proposed in similar forms a number of times [BMR97; AM00; KW08; KMP00; GM08], possibly first by Shafer and Shenoy [Sha91].

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WCSP/CFN with one variable X_i per vertex i

- Min-Cut: $D_i = \{\mathtt{l}, \mathtt{r}\}, D_s = \{\mathtt{l}\}, D_t = \{\mathtt{r}\}$ $\quad \forall (i,j) \in \boldsymbol{E}, \varphi_{ij} = \mathbf{1}(X_i \neq X_j)$
- Max-Cut: same $\quad \varphi_{ij} = \mathbf{1}(X_i = X_j)$
- Vertex Cover: $D_i = \{\mathtt{a}, \mathtt{r}\}$ $\quad \forall i, \varphi_i = \mathbf{1}(X_i = \mathtt{a}), \forall (i,j) \in \boldsymbol{E}, \varphi_{ij} = \top(X_i = X_j = \mathtt{r})$
- Max-Clique: $D_i = \{\mathtt{a}, \mathtt{r}\}$ $\quad \forall i, \varphi_i = \mathbf{1}(X_i = \mathtt{r}), \forall (i,j) \notin \boldsymbol{E}, \varphi_{ij} = \top(X_i = X_j = \mathtt{a})$
- 3-coloring: $D_i = \{\mathtt{r}, \mathtt{g}, \mathtt{b}\}$ $\quad \forall (i,j) \in \boldsymbol{E}, \varphi_{ij} = \top(X_i = X_j)$
- Min-Sum 3-coloring: $D_i = \{1, 2, 3\}$ $\quad \forall i, \varphi_i(u) = u, \forall (i,j) \in \boldsymbol{E}, \varphi_{ij} = \top(X_i = X_j)$
- ...

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

- A boolean variable x_i — per vertex $i \in V$
- A cost function $w_{ij} = w(i, j) \times \mathbb{1}[x_i \neq x_j]$ — per edge $(i, j) \in E$
- Hard edges: $w_{ij} = k$

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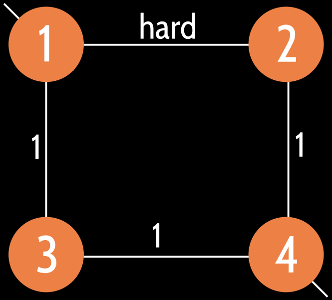
- vertices $\{1, 2, 3, 4\}$
- cut weights 1
- but edge $(1, 2)$ hard



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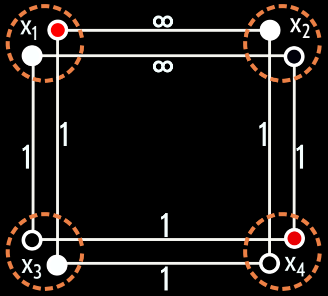

MinCut on a 3-clique with hard edge

```
{
  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: [0.0,1.0,1.0,0.0]},
      cut23:
        {scope: [x2,x3], costs: [0.0,1.0,1.0,0.0]}
  ...
}
```

The so called "local polytope" [Sch76; Kos99; Wer07] (w/o last line)

Function $\sum_{i,a} \varphi_i(a) \cdot x_{ia} + \sum_{\substack{\varphi_{ij} \in \Phi \\ a \in D_i, b \in D_j}} \varphi_{ij}(a,b) \cdot y_{iajb}$ such that

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

$$\sum_{b \in D_j} y_{iajb} = x_{ia} \qquad \forall \varphi_{ij} \in \Phi, \forall a \in D_i$$

$$\sum_{a \in D_i} y_{iajb} = x_{jb} \qquad \forall \varphi_{ij} \in \Phi, \forall b \in D_j$$

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

$nd + e.d^2$ variables. $n + 2ed$ constraints

Conditioning $\varphi_{\boldsymbol{S}}$ by $X = a \quad (X \in \boldsymbol{S})$	Assignment
Let $\boldsymbol{T} = \boldsymbol{S} - \{X\}$, this gives $\varphi_{\boldsymbol{T}}(\boldsymbol{v}) = \varphi_{\boldsymbol{S}}(\boldsymbol{v} \cup \{X = a\})$	Negligible complexity

Combination of $\varphi_{\boldsymbol{S}}$ and $\varphi_{\boldsymbol{S}'}$	Join
$(\varphi_{\boldsymbol{S}} \oplus \varphi_{\boldsymbol{S}'})(\boldsymbol{v}) = \varphi_{\boldsymbol{S}}(\boldsymbol{v}[\boldsymbol{S}]) \oplus \varphi_{\boldsymbol{S}'}(\boldsymbol{v}[\boldsymbol{S}'])$	Space/time $O(d^{\lvert\boldsymbol{S} \cup \boldsymbol{S}'\rvert})$ for tensors

Elimination of $X \in \boldsymbol{S}$ from $\varphi_{\boldsymbol{S}}$	Marginalization/Projection
$\varphi_{\boldsymbol{S}}[-X](\boldsymbol{u}) = \bigotimes_{\boldsymbol{v} \in D_X} \varphi_{\boldsymbol{S}}(\boldsymbol{u} \cup \boldsymbol{v})$	Time $O(d^{\lvert\boldsymbol{S}\rvert})$, space $O(d^{\lvert\boldsymbol{S}\rvert-1})$ for tensors

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Tree exploration — Time $O(d^n)$, linear space

- If all $|D_X| = 1, \Phi_{\mathcal{M}}(\boldsymbol{v}), \boldsymbol{v} \in D_{\boldsymbol{V}}$ is the answer
- Else choose $X \in \boldsymbol{V}$ s.t. $|D_X| > 1$ and $u \in D_X$ and reduce to
  1. one query where we condition on $X_i = u$
  2. one where u is removed from D_X
- The result of these queries is combined using $\otimes$

Optimization ($\otimes = \min$) — Branch and Bound

If a lower bound on the current query is $\succeq$ a known upper bound on $\Phi_{\mathcal{M}}$... Prune!

NB: $\varphi_{\varnothing}$ is always a lower bound.

Variable ordering

Drastic empirical effects on efficiency.

Definition (Message sent by variable X)

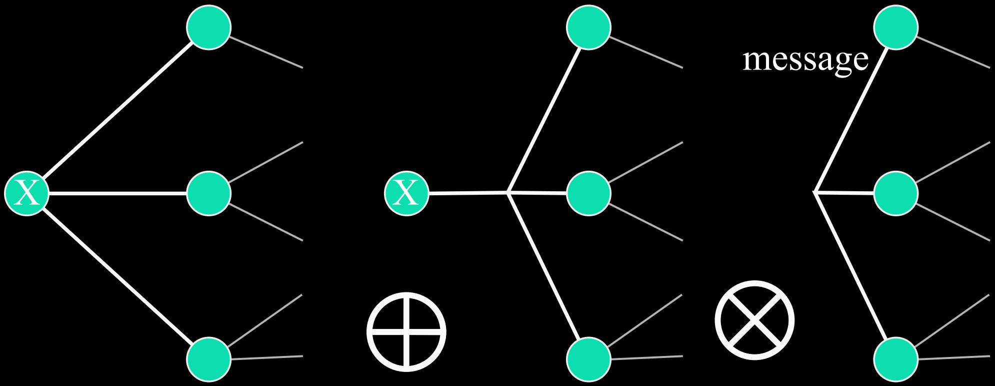
Let $X \in V$, and Φ^X be the set $\{\varphi_{\boldsymbol{S}} \in \Phi \text{ s.t. } X \in \boldsymbol{S}\}$, $\boldsymbol{T}$, the neighbors of X.

The message $m_{\boldsymbol{T}}^{\Phi_X}$ from Φ^X to $\boldsymbol{T}$ is:

$$m_{\boldsymbol{T}}^{\Phi_X} = \Big(\bigoplus_{\varphi_{\boldsymbol{S}} \in \Phi^X} \varphi_{\boldsymbol{S}} \Big)[-X] \qquad (1)$$

Eliminating a variable — Distributivity

$$\bigotimes_{\boldsymbol{v} \in D_{\boldsymbol{V}}} \left[\bigoplus_{\varphi_{\boldsymbol{S}} \in \Phi} (\varphi_{\boldsymbol{S}}(\boldsymbol{v}[\boldsymbol{S}])) \right] = \bigotimes_{\boldsymbol{v} \in D_{\boldsymbol{V}-\{X\}}} \left[\bigoplus_{\varphi_{\boldsymbol{S}} \in \Phi - \Phi^X \cup \{m_{\boldsymbol{T}}^{\Phi_X}\}} (\varphi_{\boldsymbol{S}}(\boldsymbol{v}[\boldsymbol{S}])) \right]$$


X
X
message

Complexity of one elimination for tensors

Computing $m_{\boldsymbol{T}}^{X}$ is $O(d^{|T+1|})$ time, $O(d^{|T|})$ space $|T|$ is the degree of X

The overall complexity is dominated by the largest degree encountered during elimination

Clauses $\boldsymbol{L}, \boldsymbol{L}'$ clauses

If $\Phi^X = \{(X \vee \boldsymbol{L}), (\neg X \vee \boldsymbol{L'})\}$ $m_{\boldsymbol{T}}^{\Phi X}$ is $(\boldsymbol{L} \vee \boldsymbol{L'})$.

The resolution principle [Rob65] is an efficient variable elimination process [DR94; DP60].

Dimension	induced/tree-width
Dimension of an elimination order for G	Largest set $\|T\|$ encountered
Dimension of G	minimum Dimension over all orders

Introduced in 1969 by Bertelé and Brioschi [BB69b; BB69a] (cited 19 and 31 times on GS)
Proved to be equivalent to tree-width by Bodlaender [Bod98].

The secondary optimization problem — Min degree, Minfill, MCS [Ros70]

Finding an optimal order is NP-hard, but useful heuristics exist [BK08].

Tractability

First tractable class for our general query: GMs with bounded tree-width.

Computing marginals — Stochastic Graphical Models

We want $P(X), \forall X \in \boldsymbol{V}$ — Counting

One variable X_i

- Root in X_i and eliminate all variables but X_i, from leaves.
- The elimination of X_i produces a message m_j^i involving just X_j.

All variables — Variables preserved, time & space $O(ed^2)$

Messages are kept as auxiliary functions.

- When a variable X_i has received messages from all its neighbors but one (X_j)
- Send message m_j^i to X_j

$$m_j^i = \bigotimes_{X_i}(\varphi_i \oplus \varphi_{ij} \bigoplus_{X_o \in neigh(X_i), o \neq j} m_i^o) \quad (2)$$

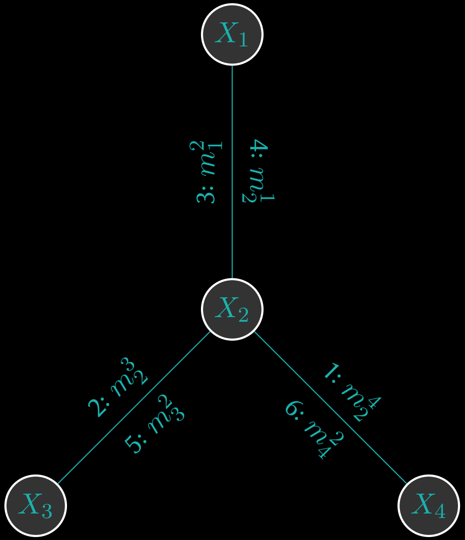


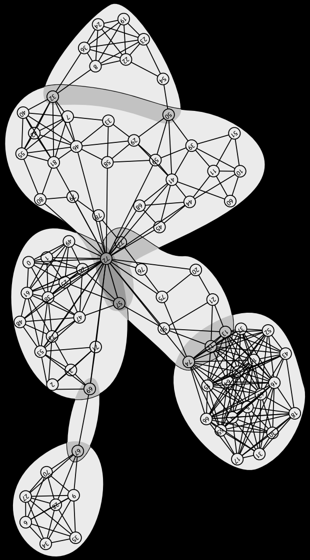
Figure 1: Message passing on a tree, a possible message schedule

The exact approach

Find a (good) tree decomposition and use the previous algorithms on the resulting tree.

Properties

- Space complexity exponential in the separator size only $\theta(d^s)$
- Many variants: block-by-block elimination [BB72], Cluster/Join tree elimination [LS88; DP89],...



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The heuristic approach

Starting from e.g., empty messages, apply the message passing equation (2)

$$m_j^i = \bigotimes_{X_i} (\varphi_i \oplus \varphi_{ij} \bigoplus_{X_o \in neigh(X_i), o \neq j} m_i^o)$$

on each function until quiescence or maximum number of iterations (synchronous or asynchronous update schemes exist).

Loopy Belief Propagation [Pea88]

- At the core of Turbo-decoding [BGT93], implemented in all cell phones.
- Widely studied [YFW01], but known to not always converge.
- Often denoted as the "max-sum/min-sum/sum-prod" algorithm.

Assume $\oplus$ is idempotent

If $\mathcal{M} = \langle \boldsymbol{V}, \Phi \rangle$ is a relaxation of $\mathcal{M}' = \langle \boldsymbol{V}, \Phi' \rangle$ then $\mathcal{M}'' = \langle \boldsymbol{V}, \Phi \cup \Phi' \rangle$ is equivalent to $\mathcal{M}'$.

Property

If $\otimes = \min$, any message $m_{\boldsymbol{T}}^{X}$ computed by elimination is a relaxation of Φ^{X} and hence of $\mathcal{M}$.

Equivalence preserving messages

- $\min - \max$ messages can be directly added to the processed graphical model
- This preserves the joint function (equivalence, so for counting too)
- Applies to Boolean, possibilistic and fuzzy structures

Variable elimination/ Resolution based

- Using variable elimination messages: David and Putnam algorithm [DP60] aka Directional Resolution [DR94].
- Using all possible messages: saturation by Resolution [Rob65].

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Definition (Arc consistency (closure property))

A graphical model $\mathcal{M} = \langle \boldsymbol{V}, \Phi \rangle$ with idempotent $\oplus$ is arc-consistent iff every variable $X \in \boldsymbol{V}$ is arc consistent w.r.t. every function $\varphi_{\boldsymbol{S}}$ s.t. $X \in \boldsymbol{S}$.

A variable X_i is arc-consistent w.r.t. a function φ_{ij} iff the message m_i^j is a relaxation of φ_i.

Arc consistency (filtering)

A graphical model $\mathcal{M} = \langle \boldsymbol{V}, \Phi \rangle$ with idempotent $\oplus$ can be transformed in polynomial time in a unique equivalent arc consistent graphical model.

Local consistency provides an incremental lower bound on consistency

If the equivalent Arc Consistent graphical model has an empty domain ($\forall a \in D_i, \varphi_i(a) = \top$), then it is infeasible/inconsistent.

Arc consistency filtering is achieved by Loopy BP

- AC-3 [Mac77] is time $O(ed^3)$, space $O(ed)$,
- AC-4 [MH86] is time $O(ed^2)$, space $O(ed^2)$,
- AC-6 [Bes94] is $O(ed^2)$, space $O(ed)$,
- AC2001/3.1 [BR01; ZY01], also optimal, empirically faster and far simpler to implement.

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Obvious issue

Without idempotency, messages can not be included in the graphical model without loosing equivalence, hence practical significance.

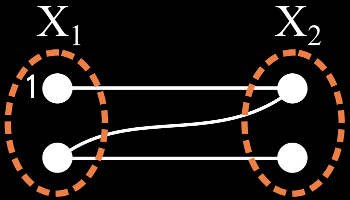
Equivalence Preserving Transformations with $\ominus$

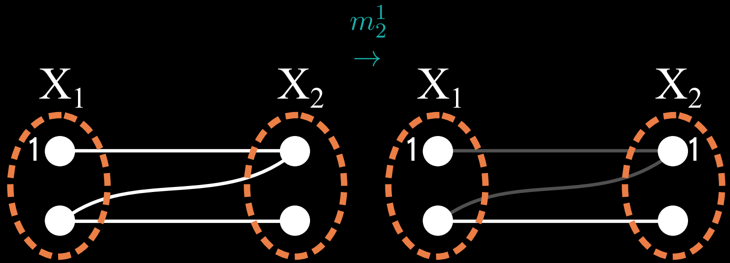
- Consider a set of functions $\Psi \subset \Phi$ and the message $m^{\Psi}_{\boldsymbol{Y}}$
- Replace Ψ by $((\bigoplus_{\varphi_{\boldsymbol{S}} \in \Psi} \varphi_{\boldsymbol{S}}) \ominus m^{\Psi}_{\boldsymbol{Y}})$ and $m^{\Psi}_{\boldsymbol{Y}}$

Any relaxation of $m^{\Psi}_{\boldsymbol{Y}}$ can be used instead.

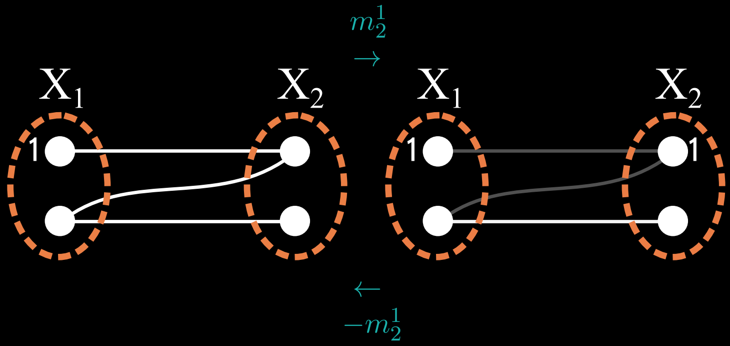
Scope preserving EPTs for tensors — Not for clauses!

If Ψ contains at most one non unary function and $|\boldsymbol{Y}| = 1$ (MRFs: reparametrizations).


X1
X2
1


m_2^1
$\rightarrow$
X_1
X_2
1
X_1
X_2
1
1

A small example that may increase $\varphi_\varnothing$



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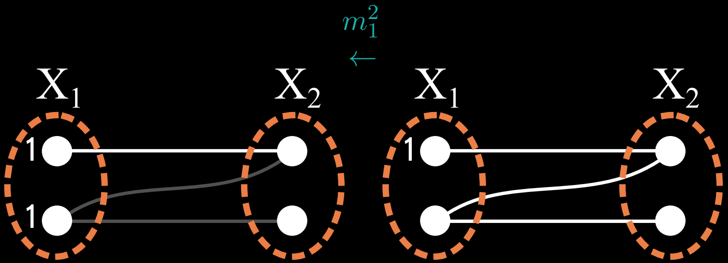
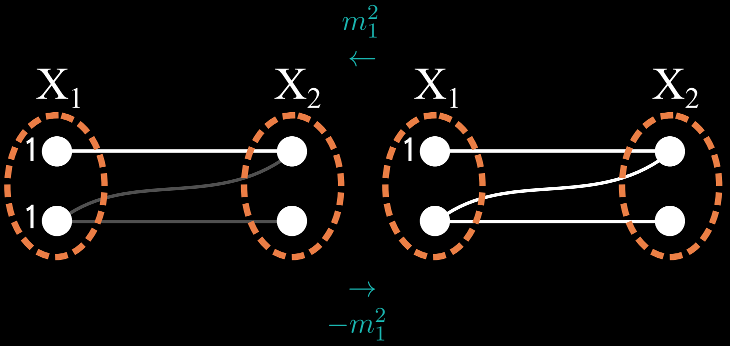
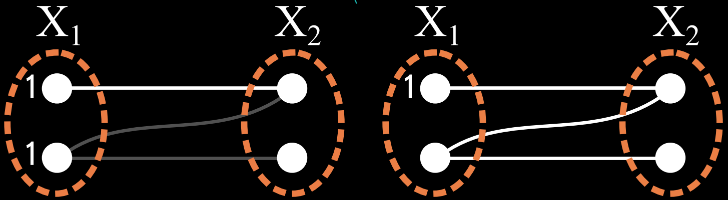



m_1^2
$\leftarrow$
X_1
X_2
1
1
X_1
X_2
1
$\rightarrow$
$-m_1^2$

A small example that may increase $\varphi_\varnothing$

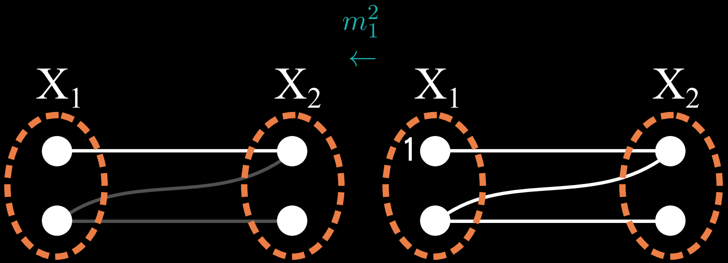
m_1^2

$\leftarrow$



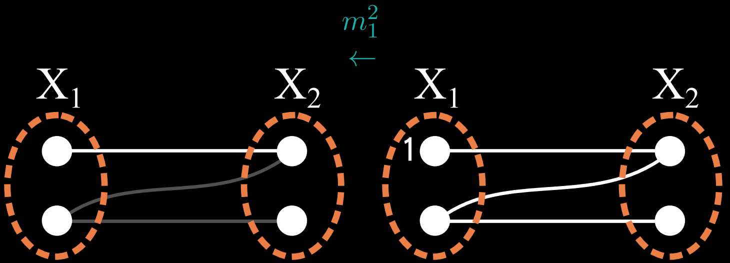
$\Downarrow \quad m_\varnothing^1$

A small example that may increase $\varphi_\varnothing$



$\Downarrow$ $m_\varnothing^1$

$\varphi_\varnothing = 1$



$\Downarrow \quad m_\varnothing^1$

$\varphi_\varnothing = 1$

(Loss of) properties

Preserves equivalence but fixpoints may be non unique (or not guaranteed to exist for some $\Psi / \boldsymbol{Y}$ configurations).

Sequence of integer EPTs

Computing a sequence of integer EPTs that maximizes $\varphi_\varnothing$ is decision NP-complete [CS04].

Set of rational EPTs (OSAC [Sch76; Coo07; Wer07])

Computing a set of rational EPTs maximizing $\varphi_\varnothing$ is in P, solvable by Linear Prog. + AC.

Essentially reduces to solving the dual of the local polytope (+ managing constraints with AC).

Universality of the Local Polytope [PW15]

Any (reasonable) LP can be reduced in linear time to a graphical model whose local polytope has the same optimum as the LP (constructive proof).

OSAC: associated polynomial classes — Empirically slow

- Tree-structured problems
- Submodular problems

Definition (Submodular function over ordered domains)

φ_S submodular if $\forall \boldsymbol{u}, \boldsymbol{v} \in D_S, \varphi_S(\min(\boldsymbol{u}, \boldsymbol{v})) + \varphi_S(\max(\boldsymbol{u}, \boldsymbol{v})) \leq \varphi_S(\boldsymbol{u}) + \varphi(\boldsymbol{v})$

Definition ($\text{Bool}(\varphi_S)$[Coo+08; Coo+10])

$\text{Bool}(\varphi_S)(\boldsymbol{u})$ is $\mathbf{0}$ iff $\varphi_S(\boldsymbol{u}) = \mathbf{0}$.

Definition ($\text{Bool}(\mathcal{M})$[Coo+08; Coo+10])

Given a weighted GM (CFN) $\mathcal{M} = \langle \boldsymbol{V}, \Phi \rangle$, the constraint network

$$\text{Bool}(\mathcal{M}) = \langle \boldsymbol{V}, \{\text{Bool}(\varphi_S) \text{ such that } |\boldsymbol{S}| > 0\} \rangle$$

Definition (Virtual Arc Consistency (VAC)[Coo+08])

A weighted GM $\mathcal{M} = \langle \boldsymbol{V}, \Phi \rangle$ is Virtual Arc Consistent iff enforcing AC on $\text{Bool}(\mathcal{M})$ does not prove inconsistency.

Algorithm loop sketch $O(ed^2k/\varepsilon)$

- Enforce AC on $\mathrm{Bool}(\mathcal{M})$
- If not proved inconsistent, done
- Extract a minimal set of messages proving inconsistency
- Apply these as EPTs on $\mathcal{M}$ (with suitable costs)
- This is guaranteed to increase $\varphi_\varnothing$

Related work

- Convergent MP in MRFs (same family of fixpoints) [Kol06; Kol15]
- Reduces to MaxFlow in the Boolean variable case
- Produces the *roof-dual* lower bound of QPBO [BH02]

Presentation Outline

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Combines — Time $O(exp(n))$

- Branch and Bound (aka Backtrack in the Boolean case)
- Incremental Local Consistency enforcing at each node (lower bound)

Variable (and value) ordering heuristics

- Crucial for empirical efficiency
- Are now adaptive (learned while searching) [Mos+01; Bou+04]
- Little theory if any.

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Additional ingredients

- Search strategies: Best/Depth First [All+15], restarts [GSC97]
- Stronger preprocessing at the root node
- Dominance analysis [Fre91; DPO13; All+14], ...

Learning from conflicts (Boolean) [Bie+09]

Extracts an informative relaxation at dead-ends using resolution (non serial DP).
Led to CDCL solvers, obsoleted DPLL (Davis, Putnam, Logemann, Loveland [DLL62]).

The power of learning [AFT11; JP12]

A randomized CDCL solver can decide the consistency of any pairwise CN instance with treewidth w with $O(n^{2w}d^{2w})$ restarts.

Pseudo-tree [Fre85; Sch99]

A pseudo-tree arrangement of a graph G is a rooted tree with the same vertices as G and the property that adjacent vertices in G reside in the same branch of the tree.

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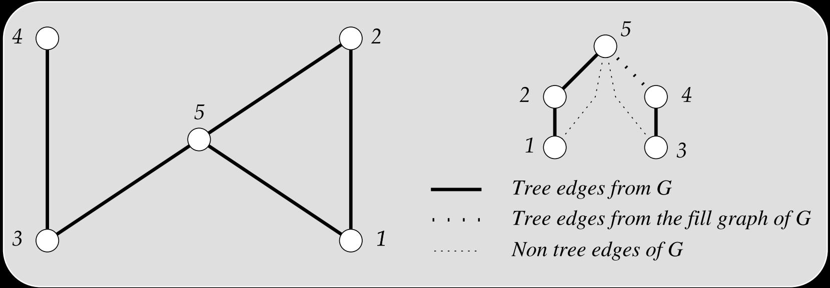

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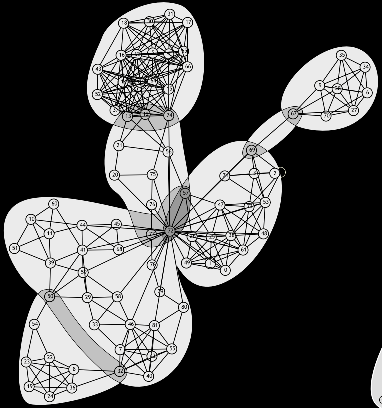

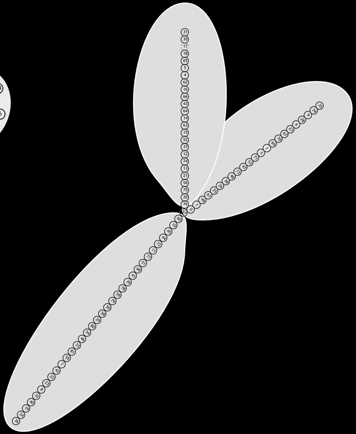

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Pseudo-tree search [Fre85]

- Solve using tree search, assigning variables from the root of the pseudo tree downwards.
- Split resolution when several connected components appear
- space efficient, time $O(exp(h))$

Pseudo-tree height h [Fre85; Sch99] $\equiv$ tree-depth [ND06]

The pseudo-tree height of G is the minimum, over all pseudo-tree arrangements of G of the height of the pseudo-tree arrangement.

Pruning using lower bounds

- AND/OR search uses mini-buckets [MD05]
- BTD uses Arc Consistency [JT03] hyper-treewidth for free [JNT08]

Caching subproblem optima (same separator assignment) time $O(exp(w))$

- AND/OR graph search [MD09]
- Backtrack with tree decompositions (BTD) [JT03; TJ03]

A difficult marriage

- Tree-decompositions constrain the variable ordering
- Variable ordering heuristics crucial for tree search

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Languages

- Boolean: A P/NP-complete dichotomy for the CSP [Bul17; Zhu17]
- Additive: the CSP dichotomy implies dichotomy for the additive case [KKR17].
- Submodularity: $\min$ and $\max$ can be replaced by any commutative, conservative functions [CCJ08].
- Finite costs: tight connection with LP [TZ16].

Hybrid tractable class — Joint Winner Property

A binary CFN satisfies the JWP iff for any three variable-value assignment, the multi-set of pairwise costs has not a unique minimum. Related to M-convex functions [TZ16].

Presentation Outline

No universal exact solver

SAT solvers: verification[1], planification, diagnosis, theorem proving,…

[1] Small neural nets too.

[2] Oliver Kullmann. “The Science of Brute Force”. In: *Communications of the ACM* (2017).

ANITI INRAE

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2017: proving an "alien" theorem? ∞

When one splits $\mathbb{N}$ in 2, one part must contain a Pythagorean triple $(a^2 = b^2 + c^2)$

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SAT solver proof[HKM16; Lam16]

$200TB$ proof, compressed to $86GB$ (stronger proof system)[2]

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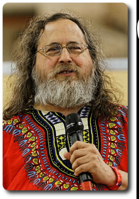
Whether it's maths or not… Size matters!

- Not only there exists true unprovable statements (in powerful enough consistent sets of axioms[Göd31])
- There may be true provable statements we will never be able to prove because of their extremely long proofs[Kul17]

A lot of free data and free code...

- International competitions ($> 50,000$ benchmarks with many real problems)
- Open source solvers (autocatalytic)



Different application areas

- CP solvers: resource management in time and or space (eg. scheduling)
- MRFs: image processing (huge problems: heuristics or primal/dual approaches, OpenGM2 [And+10], graph-cuts)
- CFNs: NLP, Computational biology, music composition, resource management (toulbar2 [Hur+16])

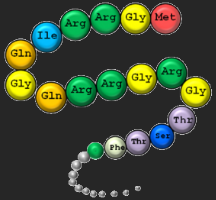
Kind words from OpenGM2 developpers

"ToulBar2 variants were superior to CPLEX variants in all our tests"[HSS18]

Most active molecules of life

Sequence of amino acids, 20 natural ones each defined by a specific flexible side-chain

Folding



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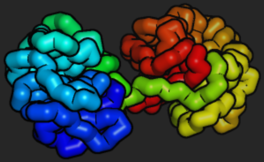


→ Function

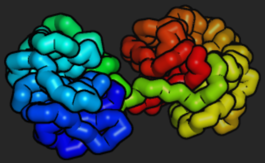
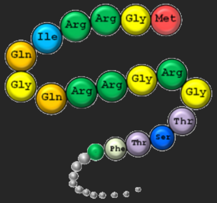
Transporter, binder/regulator, motor, catalyst…
Hemoglobine, TAL effector, ATPase, dehydrogenases…

Protein Design

Most active molecules of life

Sequence of amino acids, 20 natural ones each defined by a specific flexible side-chain

Inverse folding

Function →  → 

Transporter, binder/regulator, motor, catalyst…
Hemoglobine, TAL effector, ATPase, dehydrogenases…

Eco-friendly chemical/structural nano-agents

- Biodegradable (have been mass produced for billions of year)

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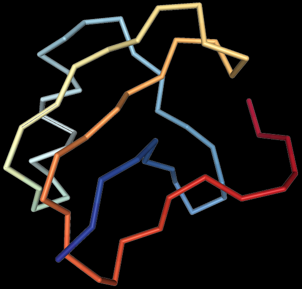
20^n sequences! intractable for experimental techniques

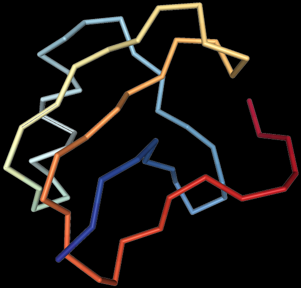
Molecular modeling

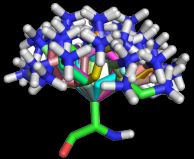
- Full atom model of a protein backbone (assumed to be rigid)



Molecular modeling

- Full atom model of a protein backbone (assumed to be rigid)
- Catalog of all side-chains in different conformations (≈ 400 overall)





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Molecular modeling

- Full atom model of a protein backbone (assumed to be rigid)
- Catalog of all side-chains in different conformations ($\approx$ 400 overall)
- Sequence-conformation space: 400^n (or more)
- Approximate decomposable energy function (intermolecular force field)

Central problem	(plenty of tricky/harder variants)
Maximum stability $\equiv$ Minimum energy	NP-hard[PW02]

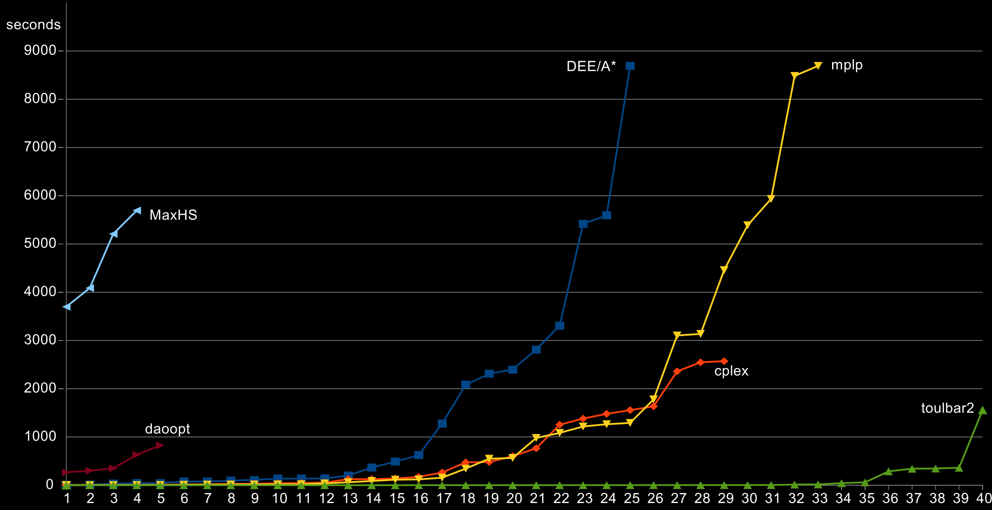
Central problem (plenty of tricky/harder variants)

Maximum stability ≡ Minimum energy NP-hard[PW02]

As a Cost Function Network[Tra+13; All+14]

- One variable per position in the protein sequence
- Domain: catalog of a few hundred amino acids conformations
- Functions: decomposed energy (pairwise terms)
- Treewidth may be less than n (depends on the protein shape)
- Empirically, functions are not permutated submodular

Toulbar2 vs. CPLEX, MaxHS...(real instances)



# of instances solved (X) within a per instance cpu-time limit (Y)

VAC vs. LP on Protein design problems

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CPLEX V12.4.0.0

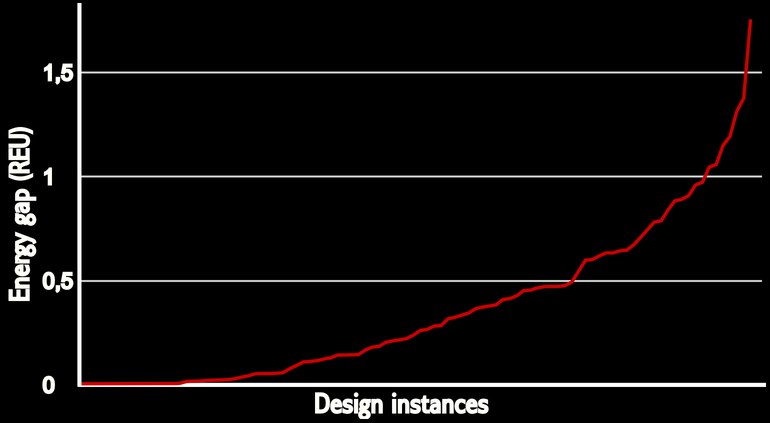
```
Problem '3e4h.LP' read.
Root relaxation solution time =  811.28 sec.
...
MIP - Integer optimal solution:  Objective =  150023297067
Solution time =  864.39 sec.
```

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.
```

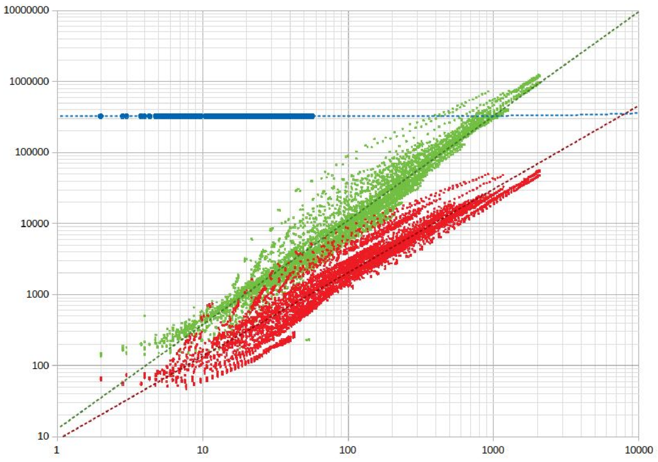
Could this be useful for ILP?

Reversing Prusa-Werner construction somehow?



Optimality gap of the Simulated annealing solution as problems get harder

Asymptotic convergence, close to infinity is arbitrarily far

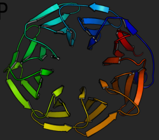


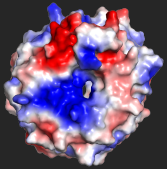
Exact vs. heuristic solvers [Mul+19]

DWave within 1.16 kcal/mol of the optimum 10% of the time, 4.35 kcal/mol 50% of the time, 8.45 kcal/mol 90% of the time.

C8 pseudo-symetric 2OVP symmetrized into a nano-component

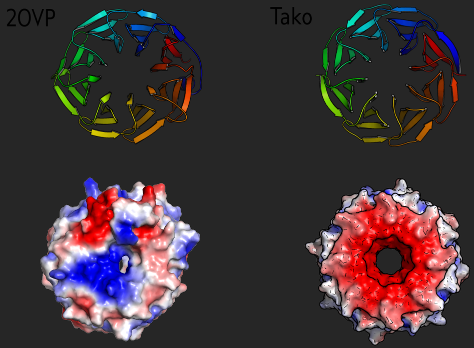
2OVP





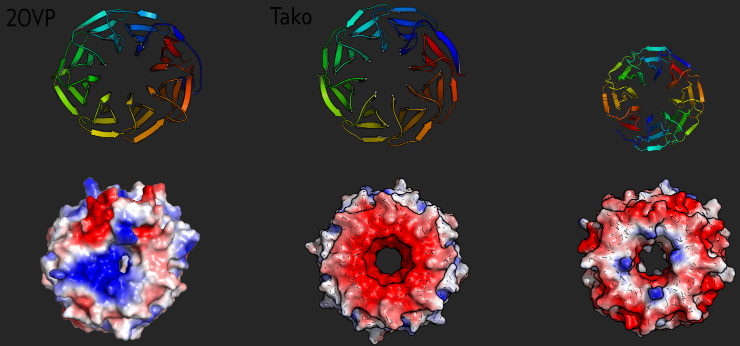
C8 pseudo-symetric 2OVP symmetrized into a nano-component

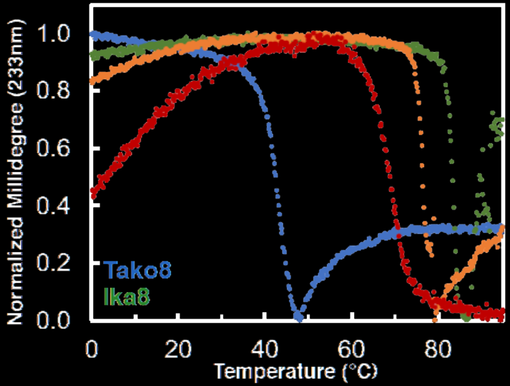
-  Tako: (R)evolution + Rosetta/talaris14 — 8 fold



C8 pseudo-symetric 2OVP symmetrized into a nano-component

-  Tako: (R)evolution + Rosetta/talaris14 — 8 fold
-  Ika: toulbar2 + talaris14 — 4 fold





Compares Tako and Ika structural stability as temperature increases (circular dichroism)

Thank You!

Questions?

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