Weighted Acyclicity Constraint for the Bayesian Network Structure Learning Problem[1]

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Overview

Bayesian Network Structure Learning

Bayesian network

is a probabilistic graphical model that captures the conditional dependencies between a set of random variables via a directed acyclic graph (DAG).

Application areas

include gene regulatory networks [Allouche et al., 2013], risk analysis [Trucco et al., 2008] and image processing [Luo et al., 2005].

Bayesian Network Structure Learning

Learning a Bayesian network

from discrete data is known to be an NP-Hard problem [Chickering et al., 2004] with an exponential search space of DAGs.

Many solution approaches

- dynamic programming [Silander and Myllymäki, 2006, Fan and Yuan, 2015]
- constraint programming [Van Beek and Hoffman, 2015]
- propositional calculus [Cussens, 2008]
- breadth-first branch-and-bound search [Campos and Ji, 2011, Fan et al., 2014]
- integer linear programming [Bartlett and Cussens, 2017].

Our Interpretation of the BNSL

CAST THE BNSL AS A COMBINATORIAL OPTIMIZATION PROBLEM

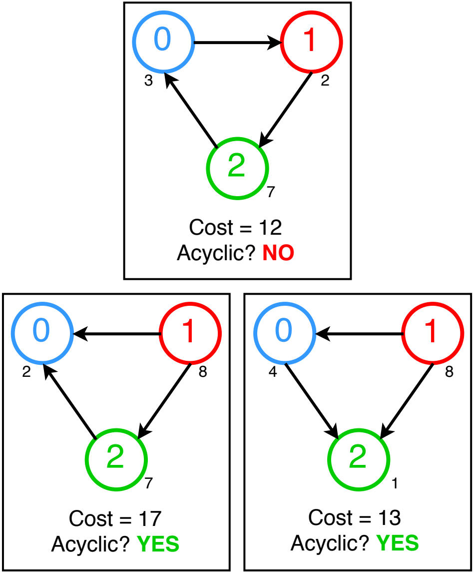
→

FORMULATE IT AS A WEIGHTED CONSTRAINT SATISFACTION PROBLEM

→

FIND AND IMPLEMENT IDEAS TO SOLVE IT FASTER

Score-and-Search Method



Variable	Parent Set	Score
0	{1, 2}	2
	{1}	4
	{2}	3
	{}	10
1	{0, 2}	1
	{0}	2
	{2}	6
	{}	8
2	{0, 1}	1
	{0}	4
	{1}	7
	{}	9

Constraint Satisfaction Problem (CSP)

A *Constraint Satisfaction Problem* [Cooper and Schiex, 2004] is a triple $\langle X, D, C \rangle$.

- X: set of n variables $X = \{1, \ldots, n\}$.
- D: set of domains $D = \{D_i : i \in X\}$.
- C: set of constraints.

Each *constraint* $c_S \in C$

is defined over a set of variables $S \subseteq X$ (its *scope*) by a subset of the Cartesian product $\prod_{i \in S} D_i = \ell(S)$. The cardinality $|S|$ is the *arity* of the constraint c_S.

A tuple $t \in \ell(X)$

is a *solution* iff it satisfies all the constraints in C.

Cost Function

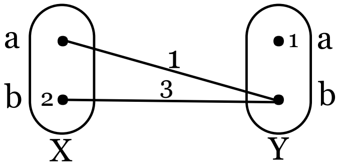
A *cost function* is defined over the scope S of the constraint c_S to which it corresponds. It associates a cost to each tuple $t \in \ell(S)$.

- $c_\varnothing$: the nullary cost function = constant cost.
- c_i: the unary cost function on variable i.
- c_{ij}: the binary cost function on variables i and j.

x	c_x
a	0
b	2

y	c_y
a	1
b	0

x	y	c_{xy}
a	a	0
a	b	1
b	a	0
b	b	3



Weighted Constraint Satisfaction Problem

Weighted Constraint Satisfaction Problem (WCSP)

is a quadruple $\langle X, D, C, m \rangle$ where C is a set of cost functions and m is the *upper bound* [Cooper et al., 2010].

Find a solution such that the sum

$$c_{\varnothing} + \sum_{i \in X} c_i + \sum_{ij \in X^2} c_{ij}$$

- is minimized,
- is less than the upper bound m.

Levels of Local Consistency

Node Consistency

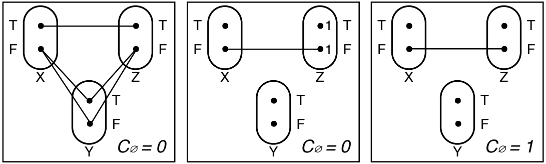
A WCSP is *node consistent* (NC) [Cooper et al., 2010] if for any variable $i \in \{1, \ldots, n\}$,

1. $\forall a \in D_i, c_i(a) \oplus c_\varnothing < m$
2. $\exists a \in D_i$ such that $c_i(a) = 0$

(Soft) Arc Consistency

A binary WCSP is arc consistent if for all $c_{xy} \in C$ we have:

$$\forall a \in D_x,\ \exists b \in D_y \text{ such that } c_{xy}(a, b) = 0.$$



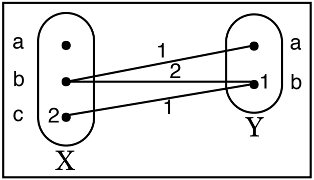
Levels of Local Consistency

Bool(P)

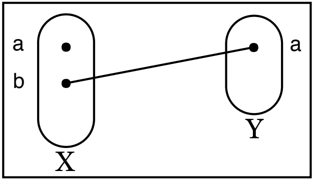
If $P = \langle X, D, C, m\rangle$ is a WCSP, then $Bool(P) = \langle X, D, \overline{C}\rangle$ is the classical CSP where, for all scopes $S \neq \varnothing$, $\langle S, R_S\rangle \in \overline{C}$ iff $\exists\langle S, c_S\rangle \in C$, where R_S is the relation defined by $\forall x \in \ell(S)\ (t \in R_S \Leftrightarrow c_S(t) = 0)$.

Virtual Arc Consistency

A WCSP P is *virtual arc consistent* (VAC) if $Bool(P)$ is arc consistent.



P



Bool(P)

Bayesian Network Structure Learning as a WCSP

Set	Variable	Domain	Unary Cost
P	P_i	Some subsets of $X \backslash i$.	Scores.
E	E_{ij}	0	0
		1	0
B	B_{ij}	0	0
		1	m if $i = j$, 0 otherwise.

Table: Decision variables.

Constraints

- *P_i and E_{ij}:* For all $i, j \in X$, we have $E_{ji} \Leftrightarrow (j \in P_i?)$.
- *E_{ij} and B_{ij}:* For all $i, j \in X$, we have $E_{ij} \Rightarrow B_{ij}$.
- *B_{ij}'s:* For all $i, k, j \in X$, we have $(B_{ik} \wedge B_{kj}) \Rightarrow B_{ij}$, which is equivalent to $\overline{B_{ik}} \vee \overline{B_{kj}} \vee B_{ij}$.
- *Enforcing acyclicity:* For all $i, j \in X$, we have $B_{ii} = 0$.

P_i vs E_{ji}		
$j \in P_i?$	Eji	Cost
0	0	0
0	1	m
1	0	m
1	1	0

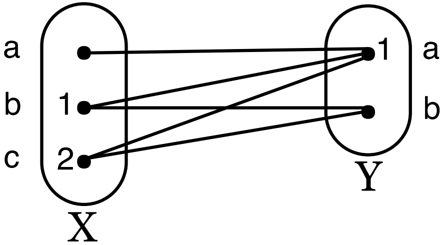
E_{ij} vs B_{ij}		
E_{ij}	B_{ij}	Cost
0	0	0
0	1	0
1	0	m
1	1	0

Table: Table costs.

Strict Arc Consistency

A variable $x \in X$ is *strictly arc consistent* if there exist values $a \in D_x$ and $b \in D_y$ for all $y \in nb(x)$ such that:

- $c_x(a) < c_x(i) \; \forall i \in D_x \backslash a$
- $c_{xy}(a, b) < c_{xy}(i, j) \; \forall (i, j) \in \ell(\{x, y\}) \backslash (a, b)$.



$x = a$ and $y = b$ is obviously the optimal assignment.

Strict Arc Consistency

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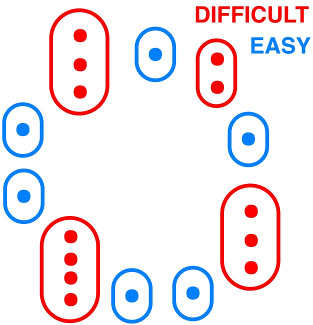


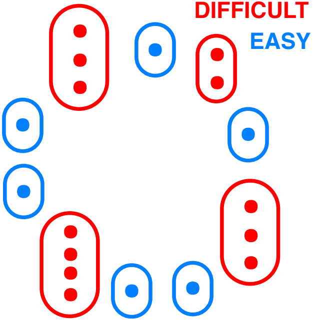
Decomposing the Problem

[Savchynskyy et al., 2013] suggests a method for energy minimization for Markov random fields:

- Divide the problem into two: easy and difficult, to be treated by convex and combinatorial techniques, respectively.

- Easy part is strictly arc consistent, while the difficult part is the rest.

- Use a similar idea for the *Bool*(P) to improve the choice of variables during Branch-and-Bound.



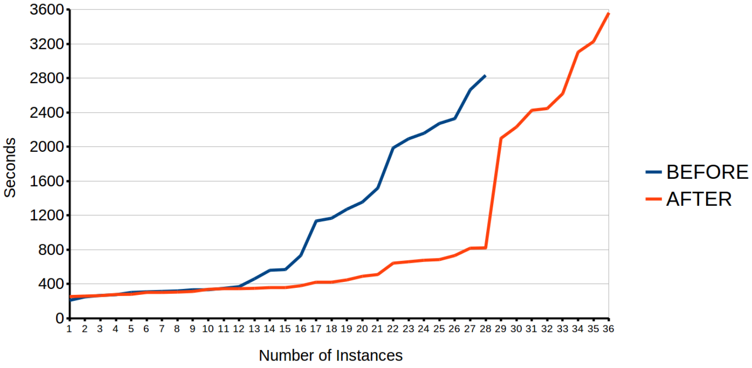
Experiments

- ToulBar2: an open-source exact solver for cost function networks that solves various combinatorial optimization problems.

- 60 instances from [Haller et al., 2018]

- Time limit: 3600 seconds

Numerical Results



Future Work

- Heuristics:
  - Stronger detection of tractable part of Bool(P)
- BNSL:
  - Improve complexity of each iteration of VAC
  - Dynamic computation of parent sets (exponentially large domains)

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