

Exact Structure Learning of Bayesian Networks

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Outline



- Background on Structure Learning as an Optimization task
- 2 Integer linear programming approach
- Dynamic programming approach
- 4 Constraint programming approach
- 5 Comparative Results
- 6 Conclusions

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• Joint probability distribution over random variables

- Finite set V of p variables
- Finite domains for each discrete variable

e.g., p = 3 genes $V = \{A, B, C\}$ with domains $\{false, true\}$, construct a Bayesian network that represents P(A, B, C)

Defines a set of conditional (in)dependencies
 e.g., A ⊥⊥ B, A ⊥⊥ B|C, ...

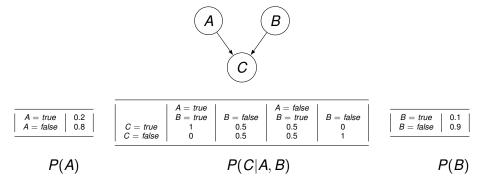
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- Equivalent to a product of conditional probabilities
 e.g., P(A, B, C) = P(A)P(B)P(C|A, B)
 - One term per variable
 - Must sum to one: $\sum_{A} \sum_{B} \sum_{C} P(A, B, C) = 1$
 - Compact formulation
 - Only some (in)dependencies can be expressed

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Equivalent to a compact representation by a

- Directed acyclic graph (DAG)
- Conditional probability tables (CPT)



- Expert knowledge
- Learning BN structure from data
 - We will assume complete data (no missing values)
 - Independent and identically distributed sample data

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Different approaches

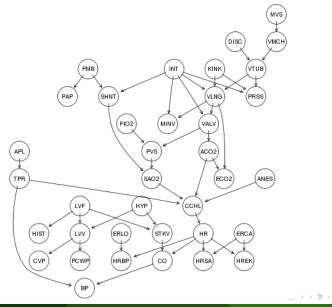
 Statistical independence tests PC [Spirtes, Glymour and Scheines, 1993],...

Search and score

Hill-Climbing [Chickering et al, 1995], GES, LAGD, Stochastic Greedy Search (SGS³) [Vandel et al., 2012a],...

Hybrid approaches Max-Min Hill-Climbing (MMHC) [Tsamardinos et al, 2006],...

Bayesian network Alarm (p = 37, 46 arcs)



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Stochastic Greedy Search [Vandel et al., 2012a]

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		Alarm			SURANG		
Nombre d'observation	s 50	500	5k	50	500	5k	
SGS ¹ FP	44	10	10	18	5	3	-
FN	14	4	2	32	20	10	
SGS ² FP	44	10	10	18	5	3	
FN	14	4	2	32	20	9	
SGS ³ FP	44	8	6	19	4	1	
FN	14	3	2	32	20	8	
LAGD FP	31	11	8	15	4	5	
FN	14	4	2	32	20	11	
GES FP	18	6	4	12	2	3	
FN FN	19	5	2	34	23	12	
	H	AILFINE	DER	1	Pigs		
SGS ¹ FP	18	17	16	558	36	49	-
FN FN	43	24	14	281	0	0	
SGS ² FP	18	17	16	560	34	49	
FN	43	24	13	284	0	0	
SGS ³ FP	18	17	16	587	32	41	
FN	43	24	13	281	0	0	
IACD FP	17	21	20	n/a	n/a	n/a	
LAGD FN	42	26	19	n/a	n/a	n/a	
CES FP	15	15	11	121	2	0	
GES FN	43	24	22	420	7	0	
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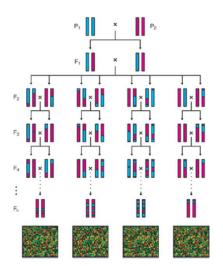
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Genetical genomics

Gene-expressions vary due to polymorphisms (stationary phenomenon in controlled environment)

Data

- gene-expression levels
- marker genotypes
- marker/gene localisations on the genome



[Jansen and Nap, Trends in Gen., 2001]

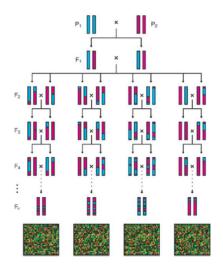
Genetical genomics

Gene-expressions vary due to polymorphisms (stationary phenomenon in controlled environment)

Data Arabidopsis thaliana

- 34,660 CATMA microarray probes
- 89 SNP marker genotypes
- marker/gene localisations on the genome

Sample size : N = 158 RIL [Loudet *et al*, Gen. 2008]



[Jansen and Nap, Trends in Gen., 2001]

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Genetical genomics on Arabidopsis thaliana

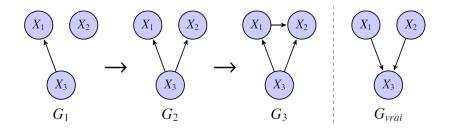
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Consensus BN 2,775 transcripts with high eQTL (LOD > 3, bootstrap > 0.3) [Vandel et al., 2012b] ~

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Wrong arc orientation issue



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Stochastic Greedy Search with post-processing [Vandel et al., 2012a]

		Alarm			INSURANCE		
Nombi	Nombre d'observations		500	5k	50	500	5k
SGS ¹	FP	39	8	5	17	5	3
202	FN	15	4	2	32	21	10
SGS ²	FP	39	7	5	17	4	3
202-	FN	15	4	2	32	20	9
SGS ³	FP	40	6	2	17	4	1
202	FN	14	3	2	32	20	8
GES	FP	18	6	4	12	2	3
UE2	FN	19	5	2	34	23	12
		HA	AILFIND	ER	1	Pigs	
SGS ¹	FP	15	16	13	546	3	7
303	FN	43	24	14	281	0	0
SGS ²	FP	16	16	13	548	3	7
303	FN	43	24	14	284	0	0
SGS ³	FP	15	16	13	574	1	2
303	FN	43	24	13	281	0	0
GES	FP	15	15	11	121	2	0
OE2	FN	43	24	22	420	7	0

- Superexponential number of DAGs (e.g., $> 10^9$ for p = 7)
- NP-hard problem with two parents or more [Chickering, 1996]
- Various scoring functions (BIC/MDL, BDeu,...)
- Greedy search, tabu search, genetic algorithms,...
- Exact methods
 - integer linear programming [Bartlett and Cussens, 2015]
 - dynamic programming [Yuan and Malone, 2013]
 - constraint programming [van Beek and Hoffmann, 2015]

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Definition of a 0/1 Linear Program (01LP)

$\min_{x_1,x_2,\ldots,x_n}$	$\sum_{i=1}^{n}$	C _i X _i
such that	$\sum_{i=1}^{n}$	$a_{i,1}x_i \leq b_1$
	$\sum_{i=1}^{n}$	$a_{i,2}x_i \leq b_2$
		•••
	$\sum_{i=1}^{n}$	$a_{i,m}x_i \leq b_m$
	$x_i \in \{0, 1\}$	$\forall i \in \{1, \ldots, n\}$

State-of-the-art solvers : SCIP, CPLEX, Gurobi, Xpress-MP,...

- Linear relaxation *x*^{*} using continuous domains
- Cutting planes (linear inequalities implied by the problem)
- Branching

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Family 0/1 variables

Create $x_{v \leftarrow W}$ for each node $v \in V$ and candidate parent set $W \subseteq V$. $x_{v \leftarrow W} = 1$ iff W is the parent set for v.

e.g.
$$x_{A \leftarrow \emptyset} = 1$$
, $x_{B \leftarrow \emptyset} = 1$, $x_{C \leftarrow \{A,B\}} = 1$

At most $p2^{p-1}$ candidate parent sets.

In practice, we limit the number of parents per node (typically to 3 or 4).

BIC score allows at most $I = \log(\frac{2N}{\log N})$ parents for sample size *N*, ie. I = 4 for N = 450.

01LP formulation

BDeu score

We have $P(Graph|Data) \propto P(Graph)P(Data|Graph)$. P(Data|Graph) is called marginal likelihood.

BDeu score maximizes P(Data|Graph) using Dirichlet priors on the CPT parameters.

$$\begin{array}{ll} \max & \log P(Data|Graph) & = \\ & \max & \sum_{v \in \mathbf{V}} \sum_{\mathbf{W} \subseteq \mathbf{V}} c_{v \leftarrow \mathbf{W}} x_{v \leftarrow \mathbf{W}} \\ & \text{such that} & \dots \end{array}$$

Pruning can be applied on the list of candidate parent sets [de Campos and Ji, 2010] :

remove
$$x_{v \leftarrow W}$$
 if $\exists U \subseteq V, c_{v \leftarrow U} \ge c_{v \leftarrow W}$

01LP model

$$\begin{array}{lll} \max & \sum_{\nu \in \mathbf{V}} \sum_{\mathbf{W} \subseteq \mathbf{V}} c_{\nu \leftarrow \mathbf{W}} x_{\nu \leftarrow \mathbf{W}} \\ \text{such that} & \sum_{\mathbf{W} \subseteq \mathbf{V}} x_{\nu \leftarrow \mathbf{W}} = 1 & \forall \nu \in \mathbf{V} \\ & \sum_{\nu \in \mathbf{C}} \sum_{\mathbf{W} : \mathbf{W} \cap \mathbf{C} = \emptyset} x_{\nu \leftarrow \mathbf{W}} \ge 1 & \forall \mathbf{C} \subseteq \mathbf{V} \\ & x_{\nu \leftarrow \mathbf{W}} \in \{0, 1\} & \forall \nu \in \mathbf{V}, \mathbf{W} \subseteq \mathbf{V} \end{array}$$
(1)

At most $2^{p-1} - 1$ *cluster constraints* (1), Add them on-the-fly (removing one cycle/two circuits at a time)

Solve using a *branch-and-cut* method.

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Branch-and-cut

Cluster constraints

 Finding cluster C such that x* violates acyclicity the most by solving a 01LP subproblem (still NP-hard [Cussens et al., 2016])

$$\max \sum_{v \in \mathbf{V}} \sum_{\mathbf{W} \subseteq \mathbf{V}} x_{v \leftarrow \mathbf{W}}^* y_{v \leftarrow \mathbf{W}} - \sum_{v \in \mathbf{V}} z_v$$

s.t. $y_{v \leftarrow \mathbf{W}} \Longrightarrow z_v, \quad y_{v \leftarrow \mathbf{W}} \Longrightarrow \bigvee_{w \in \mathbf{W}} z_w$
$$\sum_{v \in \mathbf{V}} \sum_{\mathbf{W} \subseteq \mathbf{V}} x_{v \leftarrow \mathbf{W}}^* y_{v \leftarrow \mathbf{W}} - \sum_{v \in \mathbf{V}} z_v > -1$$

 $y_{v \leftarrow \mathbf{W}}, z_v \in \{0, 1\}$

with $y_{v \leftarrow W} \in \{0, 1\}$ for each variable $x^*_{v \leftarrow W} > 0$ and $z_v = 1$ iff v belongs to cluster **C**.

We want to add more cuts...

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Branch-and-cut

Cluster constraints

Finding clusters C corresponding to elementary circuits in a consensus directed graph G^{and} = (V, E) such that

$$(u o v) \in \mathsf{E} ext{ iff } \sum_{\mathsf{W} \subseteq \mathsf{V}: u \in \mathsf{W}} x^*_{v \leftarrow \mathsf{W}} = 1$$

e.g., $x_{C\leftarrow\{A,B\}}^* = 1, x_{B\leftarrow\{A,C\}}^* = 1, x_{A\leftarrow\{B,C\}}^* = 1$: 6 circuits of size 2 $(A \rightarrow B \rightarrow A, B \rightarrow A \rightarrow B, A \rightarrow C \rightarrow A, C \rightarrow A \rightarrow C, B \rightarrow C \rightarrow B, C \rightarrow B \rightarrow C)$ 2 circuits of size 3 $(A \rightarrow B \rightarrow C \rightarrow A \text{ and } A \rightarrow C \rightarrow B \rightarrow A)$ \implies 4 cluster constraints : • $C_1 = \{A, B\} : x_{A\leftarrow\emptyset} + x_{A\leftarrow\{C\}} + x_{B\leftarrow\emptyset} + x_{B\leftarrow\{C\}} \ge 1$ • ... • $C_4 = \{A, B, C\} : x_{A\leftarrow\emptyset} + x_{B\leftarrow\emptyset} + x_{C\leftarrow\emptyset} \ge 1$ In practice, we limit the size of the circuits (up to 6).

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Extra features

- Value Propagation : removes simple unfeasible assignments. e.g., if $x_{B \leftarrow \{A,...\}} = 1$ and $x_{C \leftarrow \{B,...\}} = 1$ then $x_{A \leftarrow \{C,...\}} = 0$
- Sink-finding Primal Heuristic (see later on dynamic programming)
- Generic cutting planes (Gomory, Strong Chvátal-Gomory, Zero-Half [Nemhauser and Wolsey, 1988])
- Set Packing Constraint $\sum_{v \in C} \sum_{W: C \setminus \{v\} \subseteq W} x_{v \leftarrow W} \le 1 \quad \forall C \subseteq V$

$$\text{e.g., } x_{A \leftarrow \{B,C\}} + x_{B \leftarrow \{A,C\}} + x_{C \leftarrow \{A,B\}} \leq 1$$

In practice, we limit to SPCs with $|\mathbf{C}| \leq 4$.

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BN datasets characteristics [Bartlett and Cussens, 2015]

Name	Equivalent Sample Size	Number of Variables	Parent Set Limit	Number of Parent Sets
car	1	7	6	35
asia	10	8	2	127
insurance	1	27	6	341
mildew	1	35	3	3520
tic-tac-toe	10	10	3	112
flag	10	30	5	24892
dermatology	10	35	3	5059
hailfinder	1	56	4	4330
kr-vs-kp	10	37	2	12877
soybean-large	2	36	2	10351
sponge	1	46	4	11042
Z00	10	18	4	6461
alarm	1	37	4	8445
diabetes	1	413	2	4441
carpo	1	60	3	16391
lung-cancer	10	57	2	8294

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Practical impact of B&C features [Bartlett and Cussens, 2015]

Network	Baseline	No Cuts of Ty	No Cuts of Type			Without Solver Feature			
		G	SCG	ZH	SPH	SPC	VP		
car	0.26 s	0.01 s	0.01 s	0.01 s	0.01 s	0.15 s	0.01 s		
asia	0.36 s	0.35 s	0.97 s	0.34 s	0.34 s	0.42 s	0.36 s		
insurance	0.83 s	0.76 s	1.00 s	0.74 s	0.81 s	1.47 s	0.81 s		
Mildew	1.20 s	1.16 s	1.16 s	1.12 s	1.21 s	2.03 s	1.21 s		
tic-tac-toe	9.40 s	5.23 s	9.18 s	2.55 s	9.26 s	8.41 s	9.30 s		
flag	39.99 s	36.79 s	17.77 s	19.14 s	36.09 s	70.85 s	35.95 s		
dermatology	32.17 s	31.19 s	21.16 s	27.49 s	31.63 s	28.84 s	29.74 s		
hailfinder	112.56 s	79.23 s	61.90 s	87.56 s	118.97 s	226.23 s	111.93 s		
kr-vs-kp	124,37 s	80.64 s	75.48 s	71.91 s	125.81 s	96.75 s	122.47 s		
soybean-large	98.41 s	92.83 s	130.14 s	82.02 s	89.90 s	110.38 s	97.14 s		
alarm	200.64 s	280.12 s	112.78 s	244.59 s	201.50 s	108.71 s	227.45 s		
Diabetes	-	-	-	-	-	-	-		
sponge	195.03 s	225.24 s	300.02 s	231.95 s	230.15 s	214.46 s	191.36 s		
Z00	264.79 s	290.40 s	191.36 s	166.54 s	266.65 s	174.74 s	214.03 s		
carpo	483.69 s	528.10 s	587.44 s	513.89 s	577.18 s	589.40 s	510.62 s		
lung-cancer	670.76 s	646.50 s	651.57 s	583,45 s	670.66 s	642.77 s	627.88 s		

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Structure Learning with dynamic programming

Key Idea

Any Bayesian network has at least one *sink* node.

 \implies choose its best parent set without introducing any directed cycle.

Recursive definition

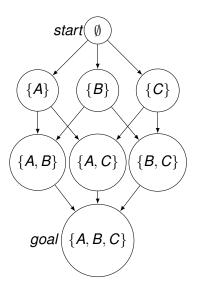
$$\log P(Data|Graph) \equiv L(\mathbf{V}) = \max_{s \in \mathbf{V}} (L(\mathbf{V} \setminus \{s\}) + \max_{\mathbf{W} \subset \mathbf{V} \setminus \{s\}} c_{s \leftarrow \mathbf{W}})$$

First, find optimal structures for single variables. Then, build optimal subnetworks for increasing larger variable sets until **V**.

Time and space complexity in $O(2^{p})$ [Silander and Myllymäki, 2006].

In practice, memory limits $p \leq 30$.

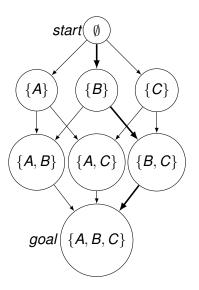
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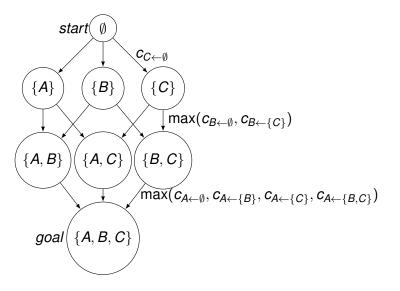
Each path from start to goal corresponds to a variable ordering

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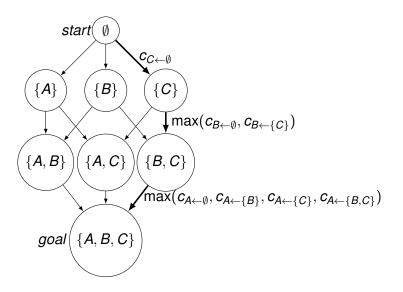
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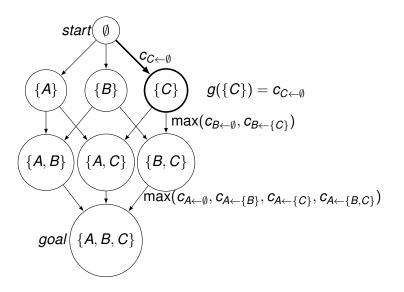
 $\mathsf{E.g.}, \emptyset \to \{B\} \to \{B, C\} \to \{A, B, C\} \text{ corresponds to order } (B, C, A) \text{ for all } (B$



Each arc $S_1 \rightarrow S_2$ has a score max_{W $\subseteq S_1 \setminus \{s\}$} $c_{s \leftarrow W}$ with $s = S_1 \cap S_2$



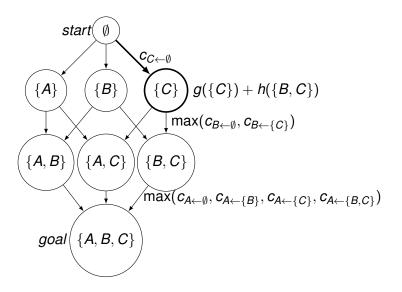
A* find an optimal path in the order graph [Yuan and Malone, 2013]



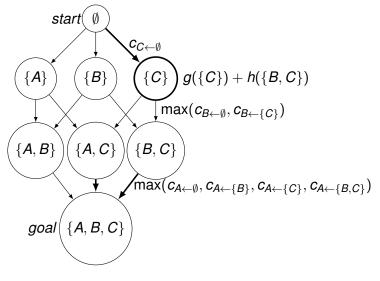
A* explores the nodes in the order graph using a best-first traversal

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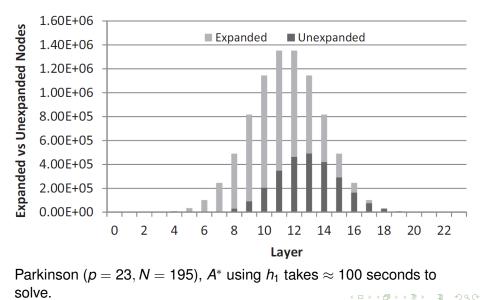
A* exploits an upper bound h on the remaining distance



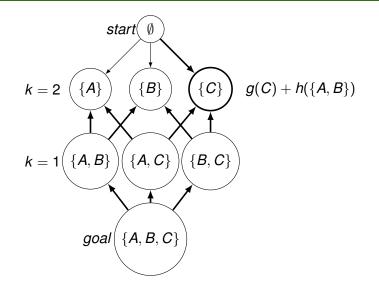
 $h_1(\mathbf{U}) = \sum_{\mathbf{v} \in \mathbf{V} \setminus \mathbf{U}} \max_{\mathbf{W} \subseteq \mathbf{V} \setminus \{\mathbf{v}\}} c_{\mathbf{v} \leftarrow \mathbf{W}}$

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Experiments with A* [Yuan and Malone, 2013]

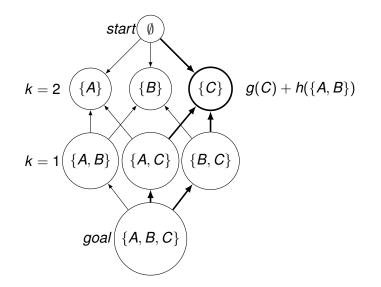


A stronger heuristic h_k for A^*



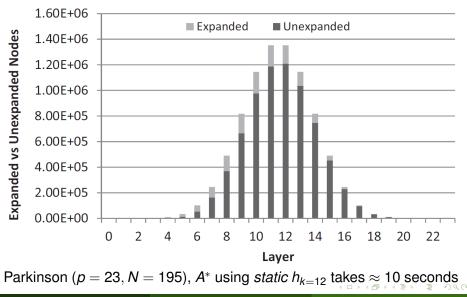
Explore from the goal up to k layers, complexity in $O(\frac{n!}{(n-k)!})$

A stronger heuristic h_k for A^*



Given a partition $\{S_1, \ldots, S_p\}$ of $V \setminus U$ with $|S_i| \le k$, $h_k(U) = \sum_{S_i} h(S_i)$

Experiments with A* [Yuan and Malone, 2013]

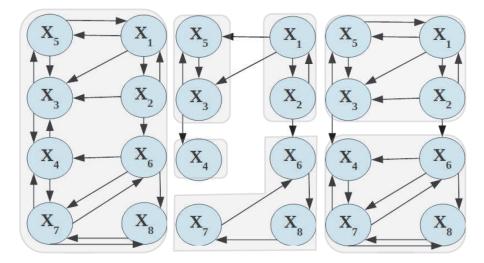


How to partition V in quasi-independent subproblems?

var.	POPS							
X_1	$\{X_2\}$	$\{X_5\}$						
X_2	$\{X_1\}$							
X_3	$\{X_1, X_5\}$	$\{X_1, X_2\}$	$\{X_2, X_4\}$	$\{X_1\}$				
X_4	$\{X_3\}$	$\{X_6\}$	$\{X_7\}$					
X_5	$\{X_1, X_3\}$	$\{X_3\}$						
X_6	$\left\{X_2, X_7\right\}$	$\{X_7\}$						
X_7	$\{X_8\}$	$\{X_6, X_4\}$						
X_8	$\{X_6\}$	$\{X_7\}$						

List of non-dominated candidate parent sets [Fan and Yuan, 2015]

How to partition V in quasi-independent subproblems?



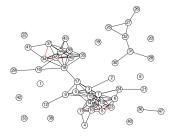
All / Top-1 / Top-2 parent relation graphs divided into SCCs [Fan and Yuan, 2015]

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Examples of parent relation graphs (BIC score)





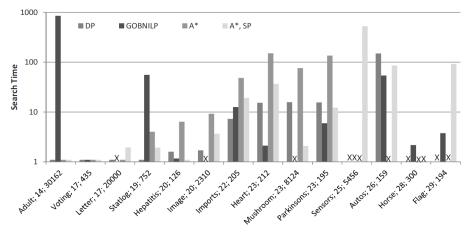
Flag (p = 29, N = 194)

Barley (p = 48, N = 1000)

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Comparative Results [Yuan and Malone, 2013]



using Minimum Description Length (~BIC) score instead of BDeu

- dual model for acyclicity : DAG encoding and topological order
- symmetry breaking constraints
- same lower bound as dynamic programming A_k^*

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Comparative Results [van Beek and Hoffmann, 2015]

			BDeu			BIC				
				GOBN.	A*	CPBayes		GOBN.		CPBayes
Benchmark	n	N	d	v1.4.1	v2015	v1.0	d	v1.4.1	v2015	v1.0
shuttle	10	58,000	812	58.5	0.0	0.0	264	2.8	0.1	0.0
adult	15	32,561	768	1.4	0.1	0.0	547	0.7	0.1	0.0
letter	17	20,000	18,841	5,060.8	1.3	1.4	4,443	72.5	0.6	0.2
voting	17	435	1,940	16.8	0.3	0.1	1,848	11.6	0.4	0.1
Z00	17	101	2,855	177.7	0.5	0.2	554	0.9	0.4	0.1
tumour	18	339	274	1.5	0.9		219	0.4	0.9	0.2
lympho	19	148	345	1.7	2.1	0.5	143	0.5	1.0	0.2
vehicle	19	846	3,121	90.4	2.4	0.7	763	4.4	2.1	0.5
hepatitis	20	155	501	2.1	4.9	1.1	266	1.7	4.8	1.0
segment	20	2,310	6,491	2,486.5	3.3	1.3	1,053	13.2	2.4	0.5
mushroom	23	8,124	438,185	OT	255.5	561.8	13,025	82,736.2	34.4	7.7
autos	26	159	25,238	OT	918.3	464.2	2,391	108.0	316.3	50.8
insurance	27	1,000	792	2.8		107.0	506	2.1	824.3	103.7
horse colic	28	300	490	2.7	15.0	3.4	490	3.2	6.8	1.2
steel	28	1,941	113,118	OT	902.9				550.8	4,447.6
flag	29	194	1,324	28.0	49.4	39.9	741	7.7	12.1	2.6
wdbc	31	569	13,473	2,055.6	OM	11,031.6	14,613		1,330.8	1,460.5
water	32	1,000					159	0.3	1.6	
mildew	35	1,000	166	0.3	7.6	1.5	126	0.2	3.6	0.6
soybean	36	266					5,926	789.5	1,114.1	147.8
alarm	37	1,000					672	1.8	43.2	8.4
bands	39	277					892	15.2	4.5	2.0
spectf	45	267					610	8.4	401.7	11.2
sponge	45	76					618	4.1	793.5	13.2
barley	48	1,000					244	0.4	1.5	3.4
hailfinder	56	100					167	0.1	9.9	1.5
hailfinder	56	500					418	0.5	OM	9.3
lung cancer	57	32					292	2.0	OM	10.5
carpo	60	100					423	1.6	OM	253.6
carpo	60	500					847	6.9	OM	OT

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- GOBNILP www.cs.york.ac.uk/aig/sw/gobnilp
- A* www.urlearning.org
- CPBayes cs.uwaterloo.ca/~vanbeek

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- A^* is limited by the number of variables (\approx 60)
- GOBNILP by the number of candidate parent sets (\approx 20,000)
- Hybrid approaches combining approximate & exact methods
- Add prior knowledge ($P(Graph|Data) \propto P(Graph)P(Data|Graph)$)
- Easy to add user constraints in generic 01LP or CP frameworks



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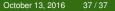


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Exact BN Learning



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