Parameterized Complexity Results for Probabilistic Network Structure Learning

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Joint work with:

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U Helsinki

Mathieu Liedloff
U d'Orleans

Sebastian Ordyniak
Masaryk U Brno

Papers:

- Algorithms and Complexity Results for Exact Bayesian Structure Learning. Ordyniak and Szeider. Conference on Uncertainty in Artificial Intelligence (**UAI 2010**).
- An Improved Dynamic Progamming Algorithm for Exact Bayesian Network Structure Learning. Ordyniak and Szeider. NIPS Workshop on Discrete Optimization in Machine Learning (**DISCML 2011**).
- On Finding Optimal Polytrees. Gaspers, Koivisto, Liedloff, Ordyniak, and Szeider. Conference on Artificial Intelligence (**AAAI 2012**).

Probabilistic Networks

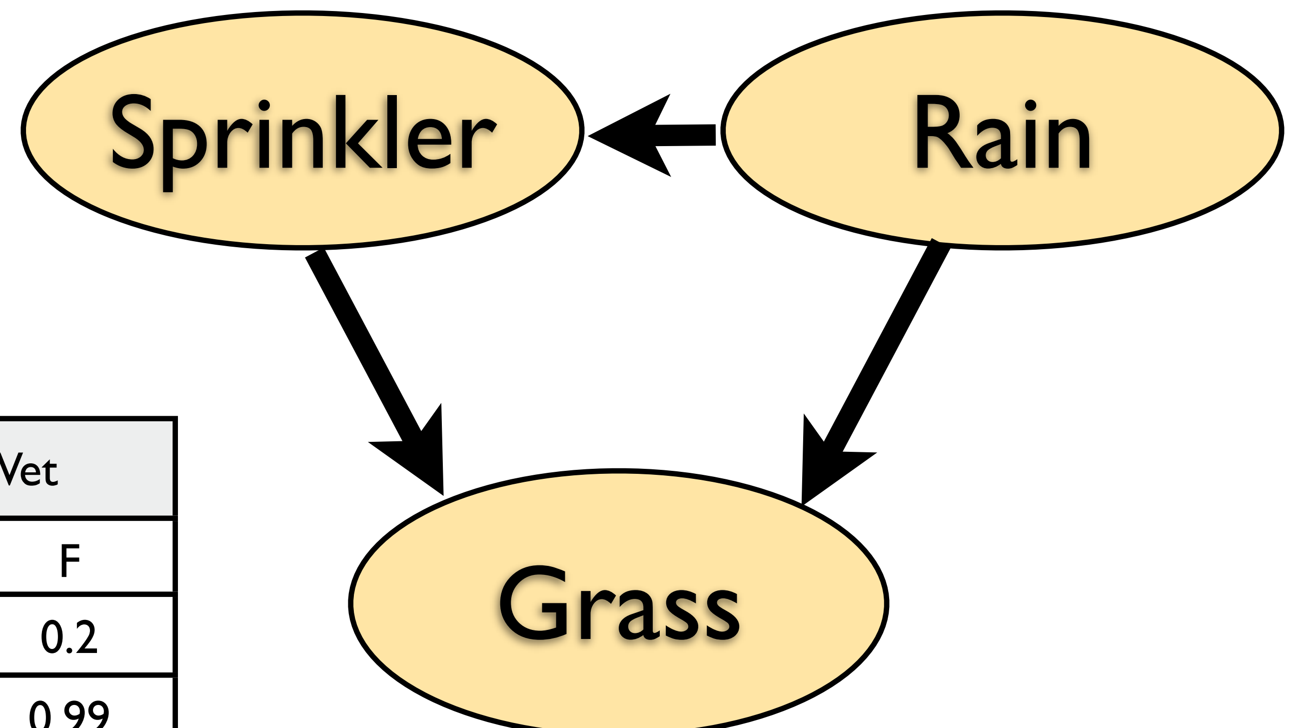
- Bayesian Networks (BNs) were introduced by Judea Perl in 1985 (2011 Turing Award Winner)
- A BN is a DAG D=(V,A) plus tables associated with the nodes of the network
- In addition to Bayesian networks, also other probabilistic networks have been considered: *Markov Random Fields, Factor Graphs*, etc.

Judea Pearl

Example: A Bayesian Network

Rain	Sprinkler	
	T	F
F	0.4	0.6
T	0.01	0.99

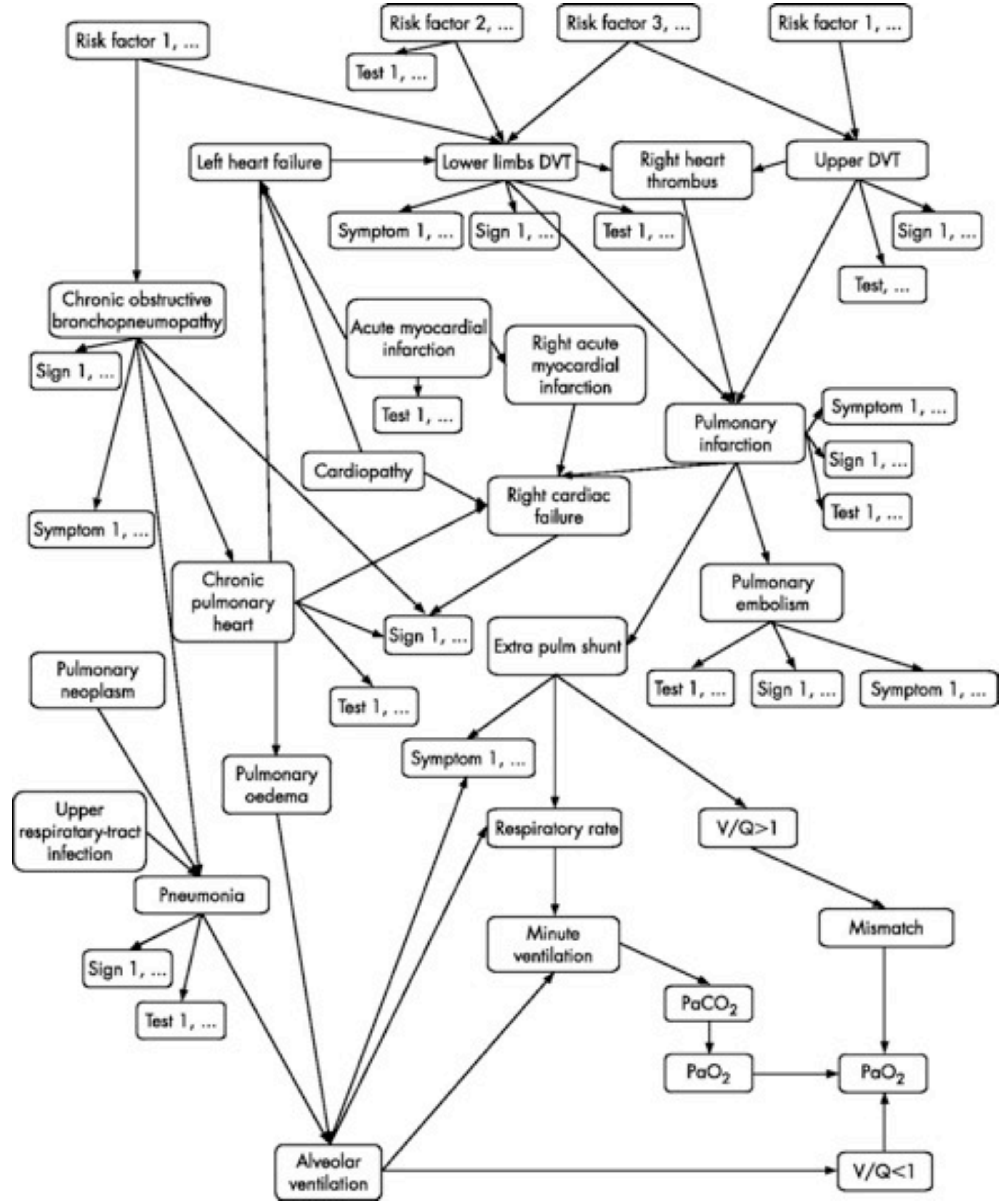
Rain	
T	F
0.8	0.2



Sprinkler	Rain	Grass Wet	
		T	F
F	F	0.8	0.2
F	T	0.01	0.99
T	F	0.9	0.1
T	T	0.99	0.01

Applications

- diagnosis
- computational biology
- document classification
- information retrieval
- image processing
- decision support
- etc.



A BN showing the main pathophysiological relationships in the diagnostic reasoning focused on a suspected pulmonary embolism event

Computational Problems

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  - BN *Parameter* Learning: Given sample data and a DAG, find the best probability tables

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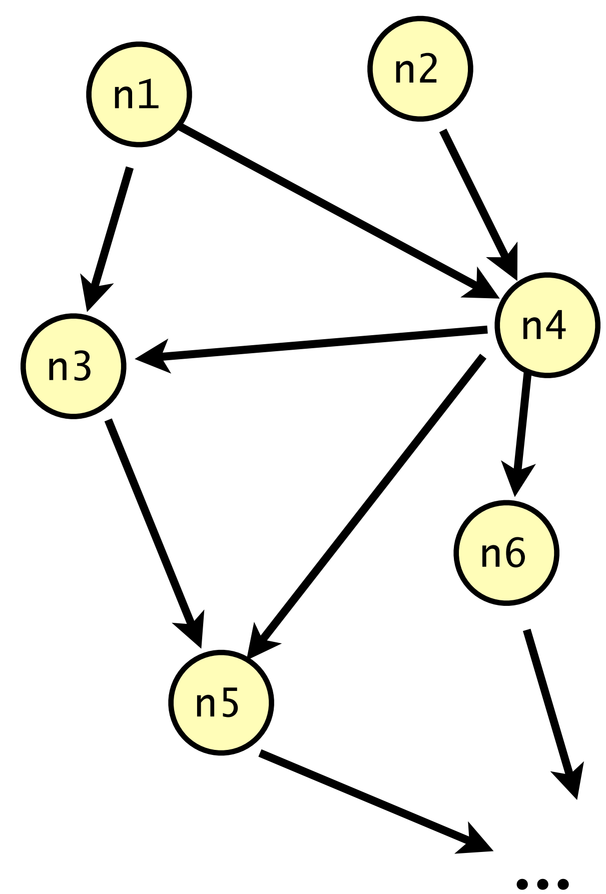
BN Learning and Local Scores

Sample Data

```
n1  n2  n3  n4  n5  n6  ....
0   1   0   1   1   0   ....
1   1   0   1   1   0   ....
*   1   0   0   *   1   ....
0   *   1   1   *   1   ....
1   0   1   1   0   1   ....
....
....
```

BN



BN Learning and Local Scores

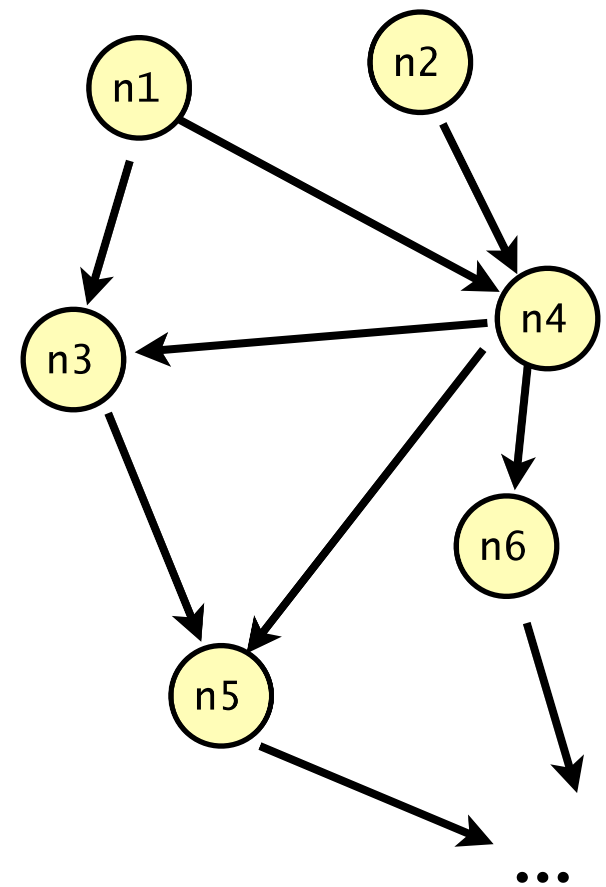
Local Score Function

f(n,P)=score of node n with P ⊆V
as its in-neighbors (parents)

Sample Data

```
n1 n2 n3 n4 n5 n6 ....
0  1  0  1  1  0  ....
1  1  0  1  1  0  ....
*  1  0  0  *  1  ....
0  *  1  1  *  1  ....
1  0  1  1  0  1  ....
....
....
```

BN



Our Combinatorial Model

- BN Structure Learning:

Input: a set N of nodes and a local sore function f (by explicit listing of nonzero tuples)

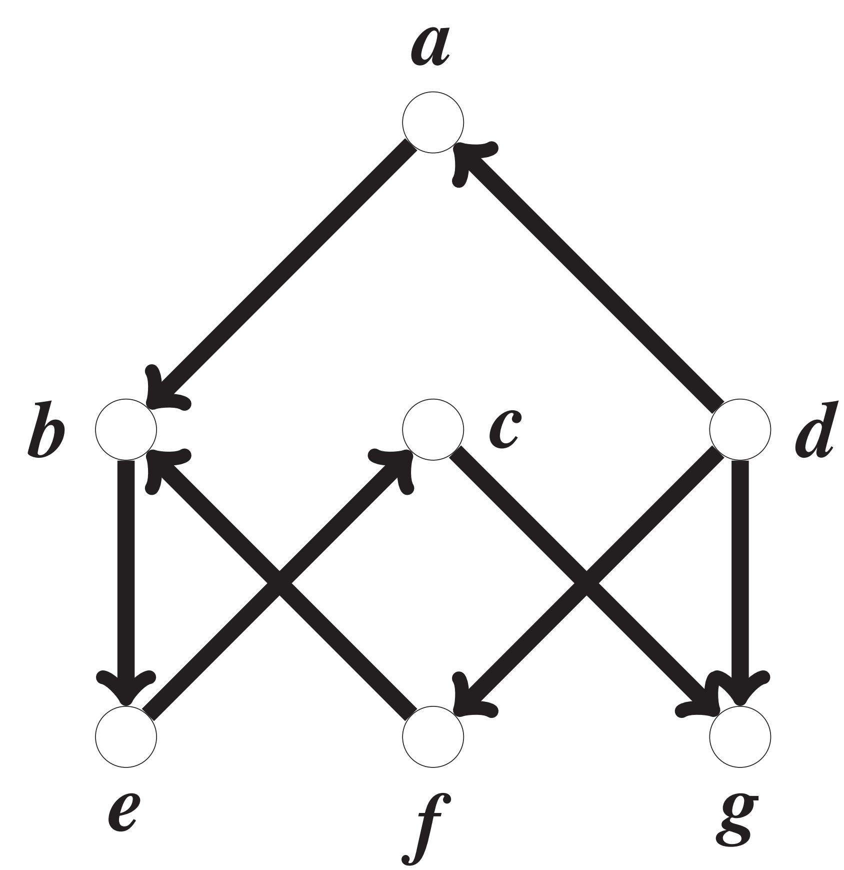
Task: find a DAG D=(N,A) such that the sum of $f(n,P_D(n))$ over all nodes n is maximum.

Example

A local score function

n	P	$f(n,P)$
a	$\{d\}$	1
a	$\{b,c,d\}$	0.5
b	$\{a,f\}$	1
c	$\{e\}$	1
d	$\emptyset$	1
e	$\{b\}$	1
f	$\{d\}$	1
g	$\{c,d\}$	1

An optimal BN structure

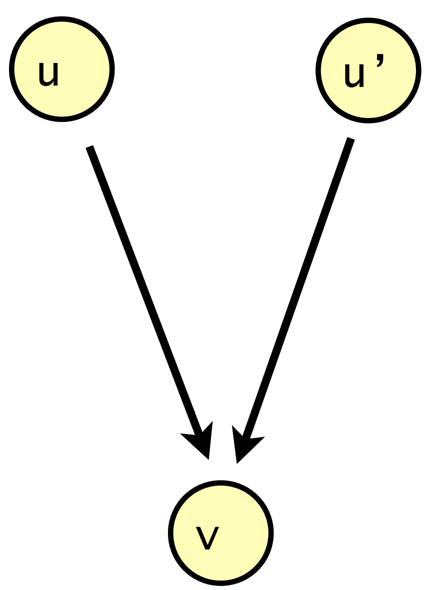


Heuristic Algorithms: find first an undirected graph, then greedily orient the edges, then do local search for improving the orientation

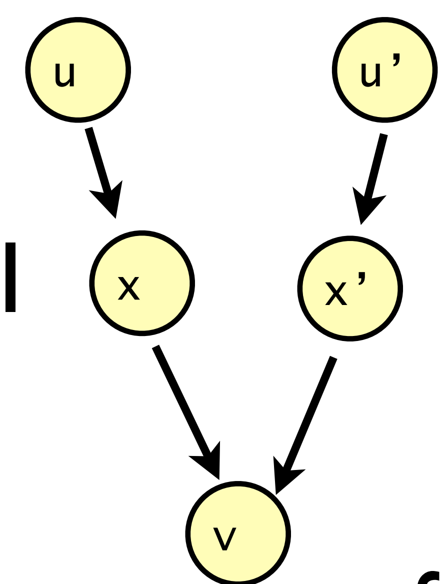
NP-Hardness

Theorem: BN Structure Learning is NP-hard.
[Chickering 1996]

- Proof: By reduction from FAS
  (NP-h for max deg 4, [Karp 1972])



$f(x,\{u\})=1$



$f(x',\{u'\})=1$

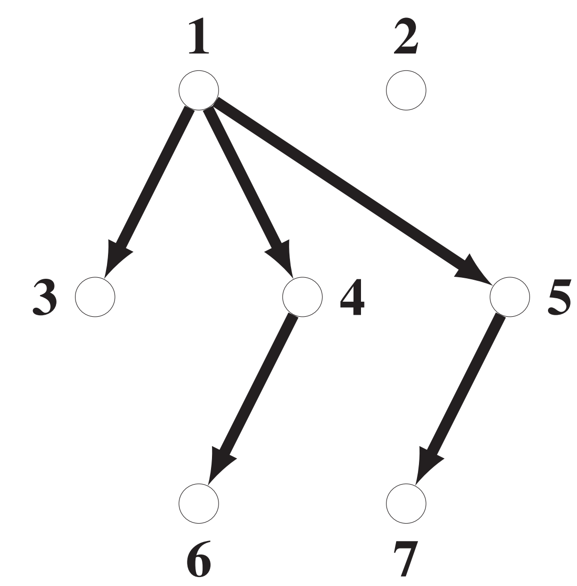
$f(v,\{x\})=1$
$f(v,\{x'\})=1$
$f(v,\{x,x'\})=2$

Very Few Polynomial Cases

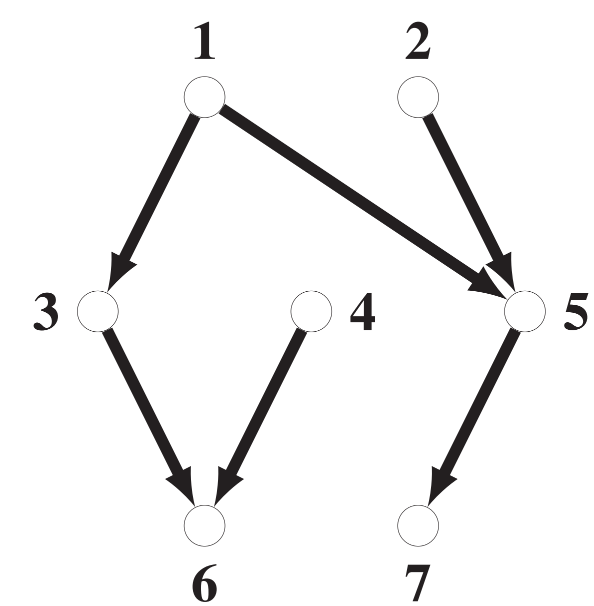
Theorem: An optimal *branching* can be found in polynomial time. (Chu and Liu 1965, Edmonds 1967)

Theorem: Finding an optimal *polytree* is NP-hard (Dasgupta 1999)

Can parameters make the problem tractable?



A branching



A polytree

Parameterized Complexity

Downey and Fellows: Parameterized Complexity Springer 1999

- Identify a parameter k of the problem
- Aim: solve the problem in time
  $f(k)n^c$
  fixed-parameter tractable (FPT)
- XP: solvable in time $n^{f(k)}$
- W-classes:
  $FPT \subseteq W[1] \subseteq W[2] \subseteq \cdots \subseteq XP$

Parameters for BN Structure Learning?

1. Parameterized by the treewidth (of the super structure)
2. Parameterized Local Search
3. Parameterized by distance from being a Branching

1.

BN Structure learning

parameterized by the treewidth

(of the super structure)

The Super Structure

- *Super structure* S_f of a local score function f is the undirected graph S_f=(N,E) containing all edges that can participate in an optimal DAG [Perrier, Imoto, Miyano 2008]

n	P	$f(n,P)$
a	$\{d\}$	1
a	$\{b,c,d\}$	0.5
b	$\{a,f\}$	1
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d	$\emptyset$	1
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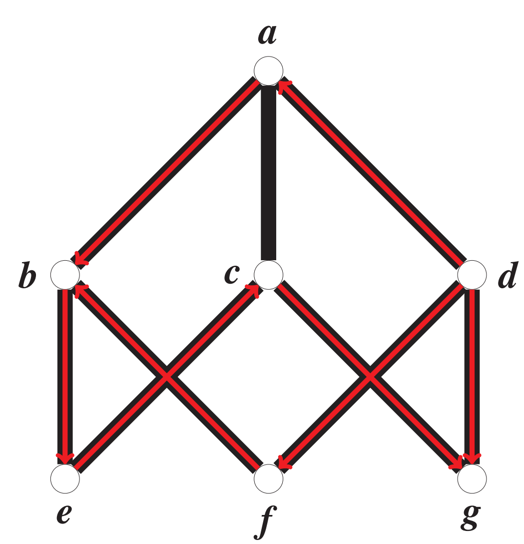
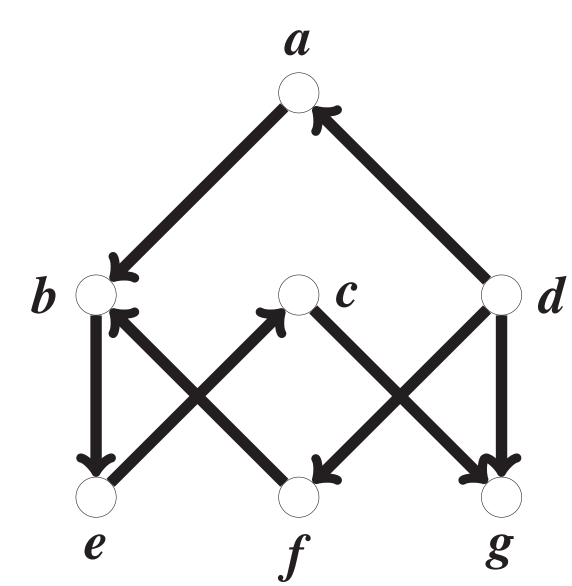
local score function



super structure



BN

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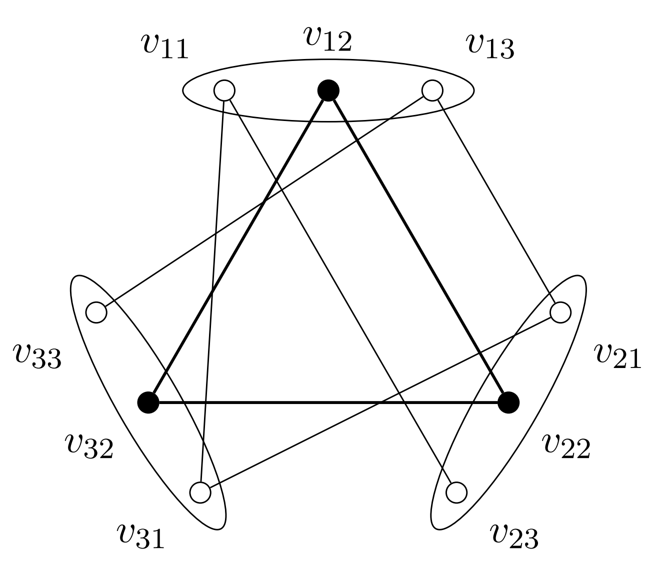

MCC instance, k=3

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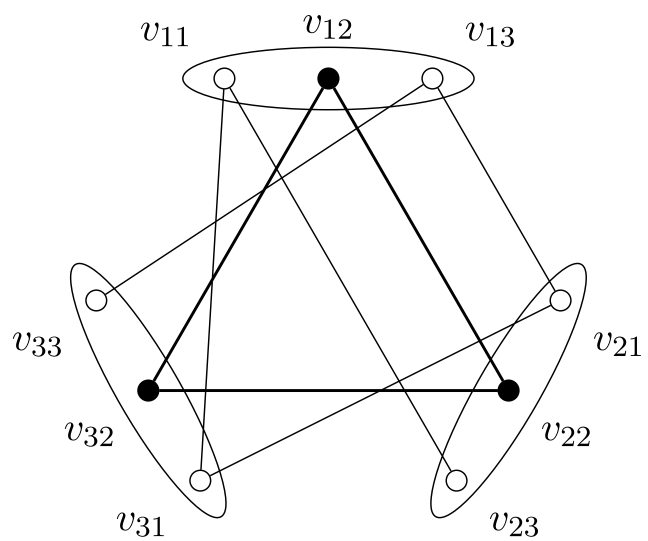

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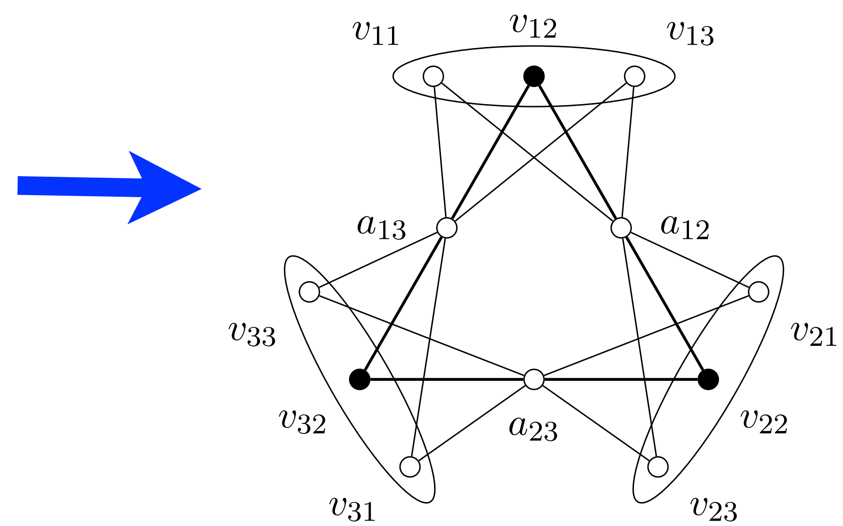

Super Structure

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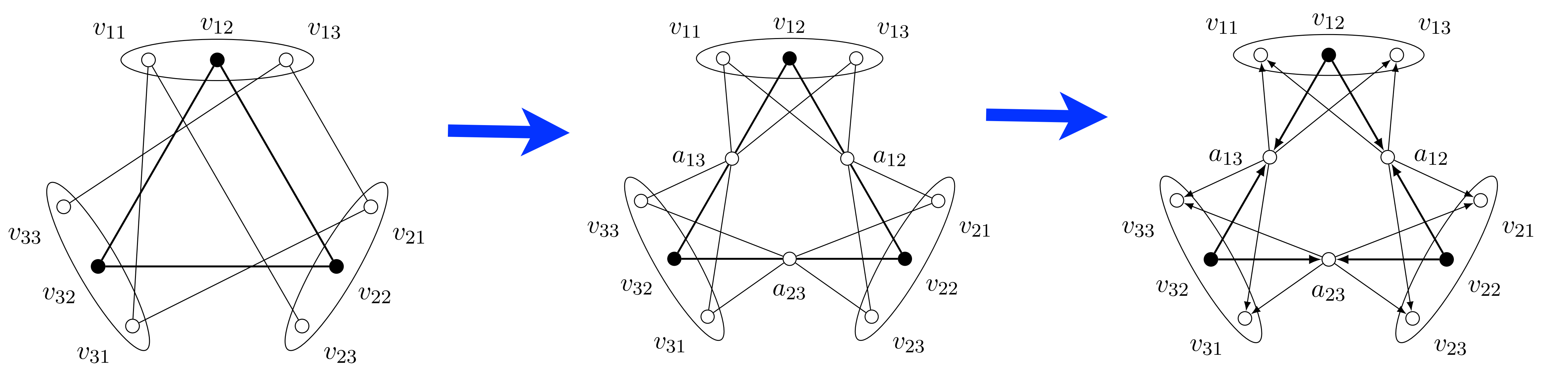

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Super Structure

BN corresponding to clique

XP-tractability

Theorem: BN Structure Learning is in XP when parameterized by the treewidth of the super structure.

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Proof: dynamic programming along a nice tree decomposition
For each node U of the tree decomp. we compute a table T(U).

T(U) gives the the highest possible score any partial solution (below U) can achieve

- for a given chosen parents of the nodes in the bag, and
- for a given reachability between nodes in the bag by directed paths.

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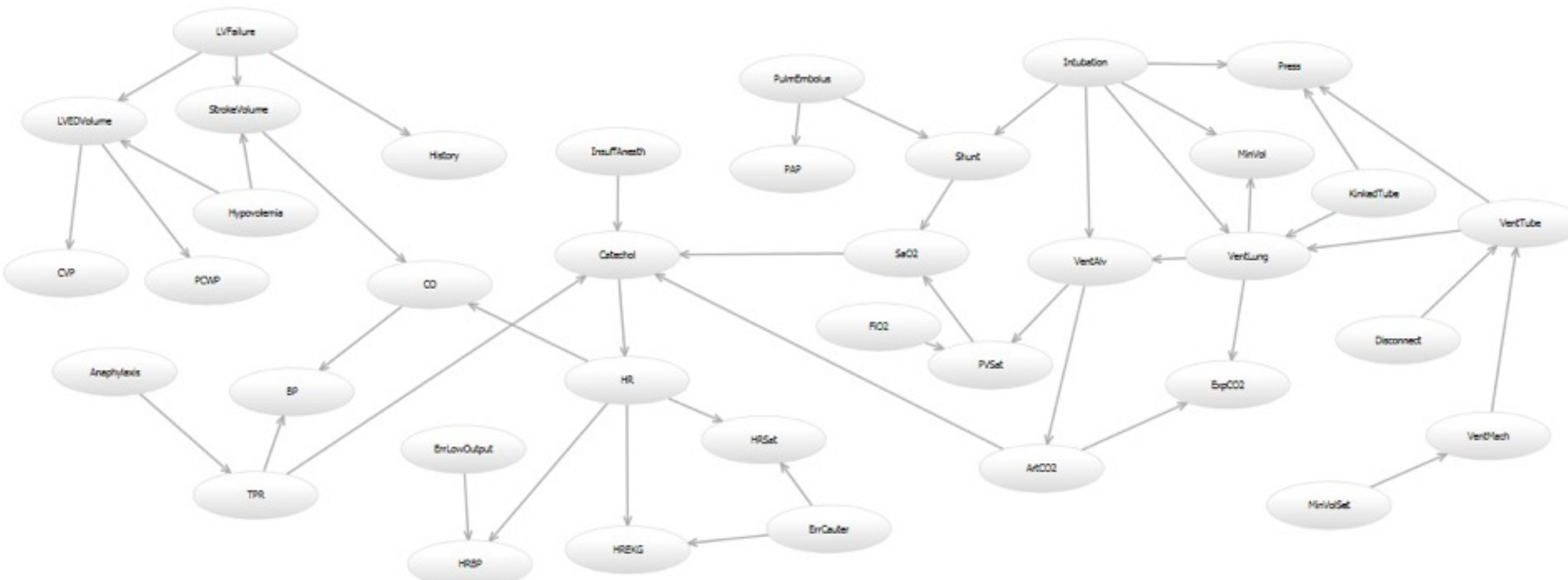
Corollary: If the super-structure has bounded degree, then we get fixed-parameter tractability

Experiments

- Alarm Network: 37 nodes



Experiments

- Bottleneck: huge tables:
- SharpLib for dynamic programming
- Dynamic Lower Bound approach (LB)
- Ongoing improvements

	Characteristics of S_f				running time (s)		memory usage (MB)	
S_f	$\|V(S_f)\|$	$\|E(S_f)\|$	$\Delta(S_f)$	$\mathrm{tw}(S_f)$	no LB	LB	no LB	LB
$\mathcal{S}_{\mathrm{SKEL}}$	37	46	6	3	14	7	337	180
$\mathcal{S}_{\mathrm{TIL}}(0.01)$	37	62	7	5	20785	6393	15679	5346
$\mathcal{S}_{\mathrm{TIL}}(0.05)$	37	63	7	5	46560	16712	38525	18786
$\mathcal{S}_{\mathrm{TIL}}(0.1)$	37	65	7	5	44554	16928	38520	18918

2.

BN Structure Learning

parameterized local search

Local Search

- Once we have a candidate BN, we can try to find a better one by local editing.
- We consider three local editing operations:
  - ADD - add an arc
  - DEL - delete an arc
  - REV - reversing an arc
- We parameterize by the number k of edits we can make in one step.

k-Local Search

- Parameterizing LS problems by the number of changes in one step has been suggested by Fellows 2003
- Since then a series of paper on that parameterized local search have been published, considering, among others: *TSP, Max-SAT, Max-Cut, Vertex Cover, Weighted SAT, Cycle Traversals, Stable Matchings*, etc.

Results

Theorem: Except for {ADD} and {DEL} all problems are W[1]-hard.

Hardness even holds for instances of bounded degree.

operations	complexity
ADD	PTIME
DEL	PTIME
REV	W[1]-h
ADD,DEL	W[1]-h
ADD,REV	W[1]-h
DEL,REV	W[1]-h
ADD,DEL,REV	W[1]-h

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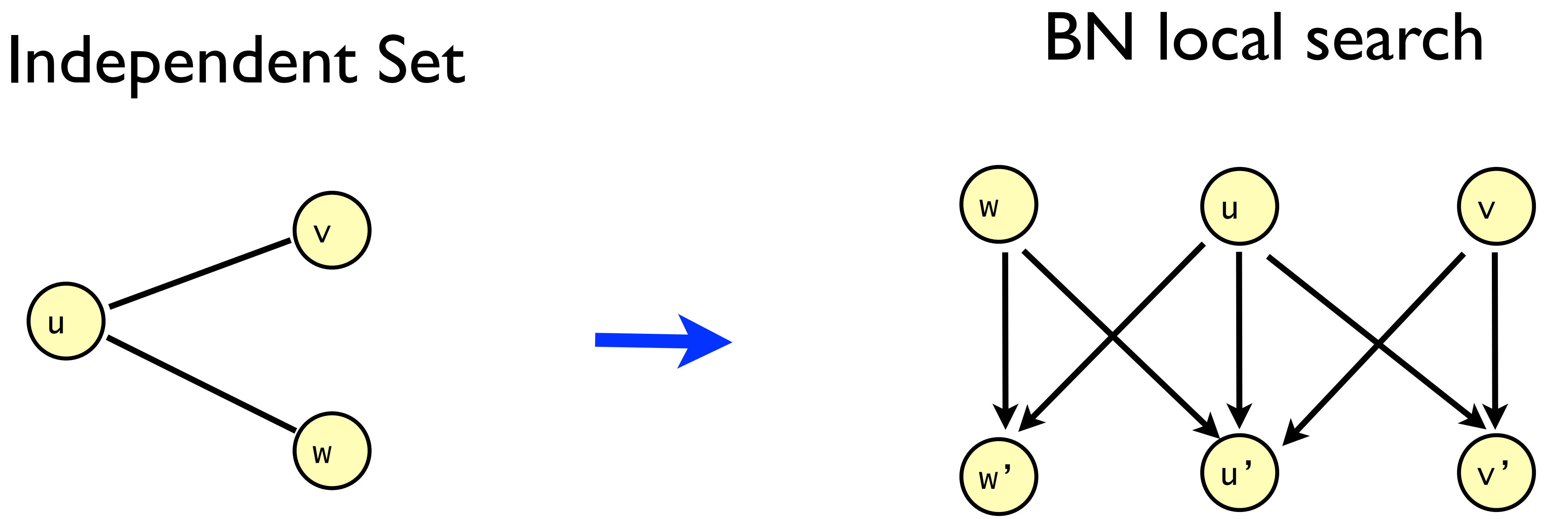
Does it help to bound the degree?

W[1]-hardness for bounded degree

- All known parameterized LS problems are FPT for instances of bounded degree.
- Almost all W[1]-hard problems are FPT for graphs of bounded degree.
- Red/Blue Nonblocker isn't an exception.
- We have now a new proof by reduction from Independent Set (we don't need the reduced graph to have bounded degree).

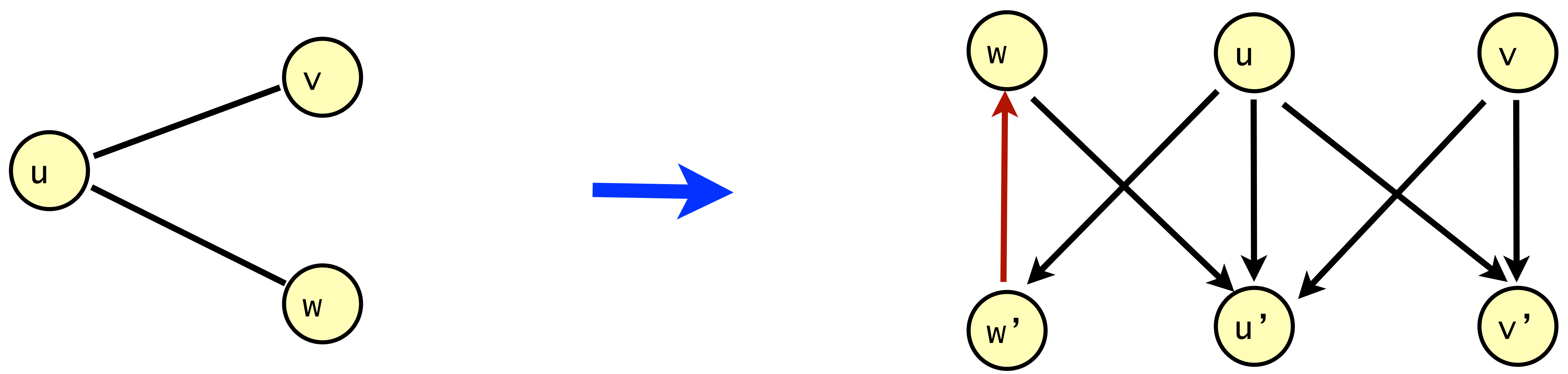
Reduction from IS for {REV}



Reduction from IS for {REV}

Independent Set

BN local search



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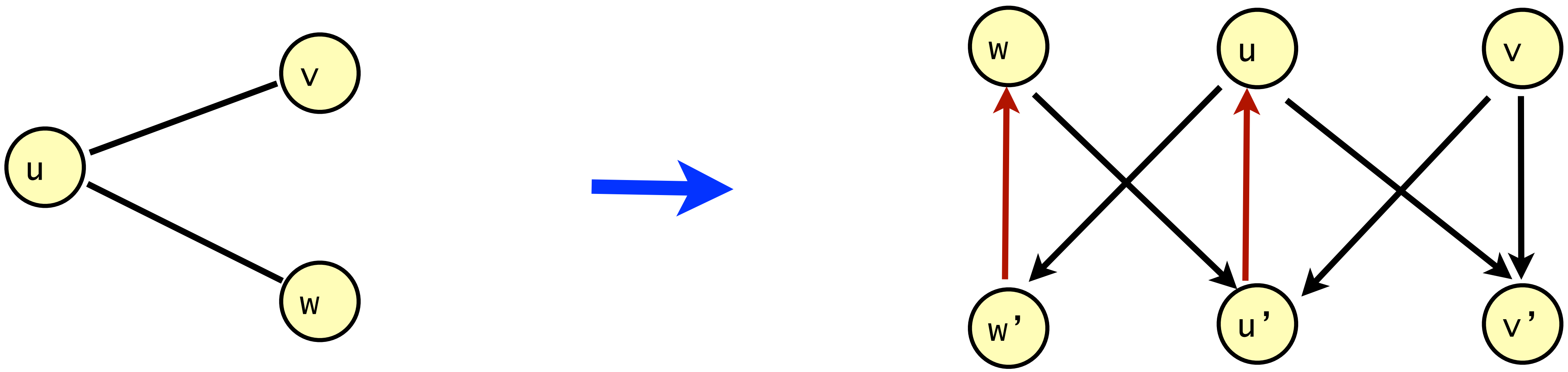

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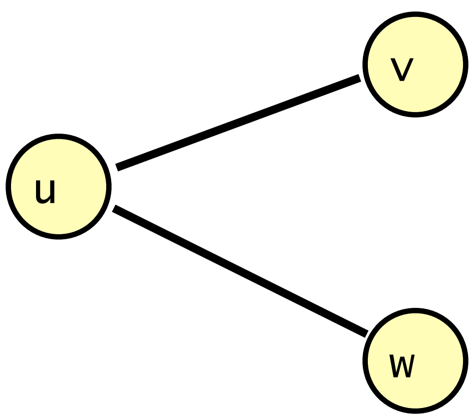
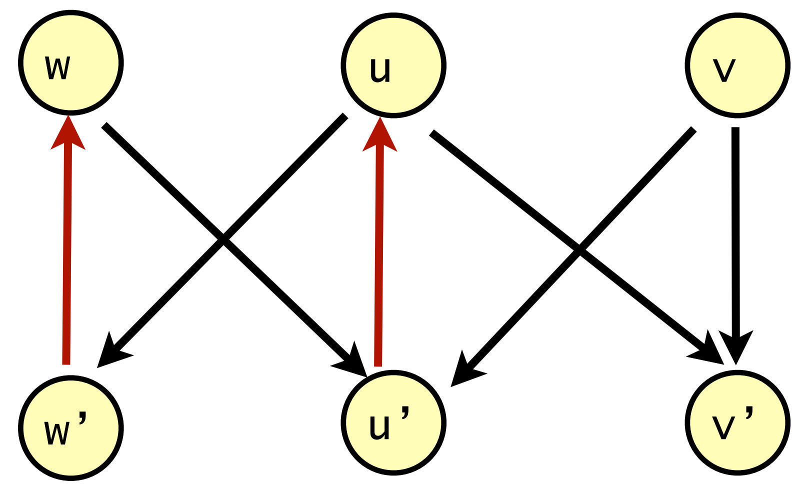
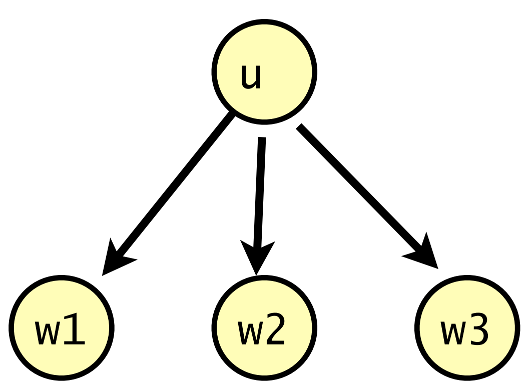
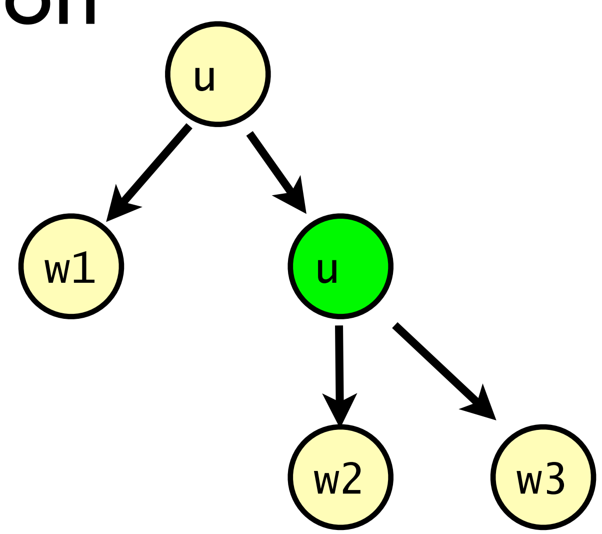


BN local search



degree reduction





3.

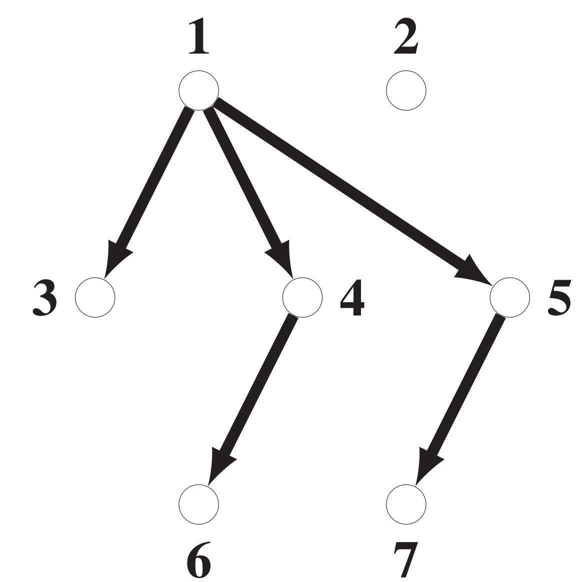
BN Structure Learning

parameterized by distance from being a branching

Beyond Branchings

Beyond Branchings

Theorem: An optimal *branching* can be found in polynomial time.
[Chu and Liu 1965, Edmonds 1967]



A branching

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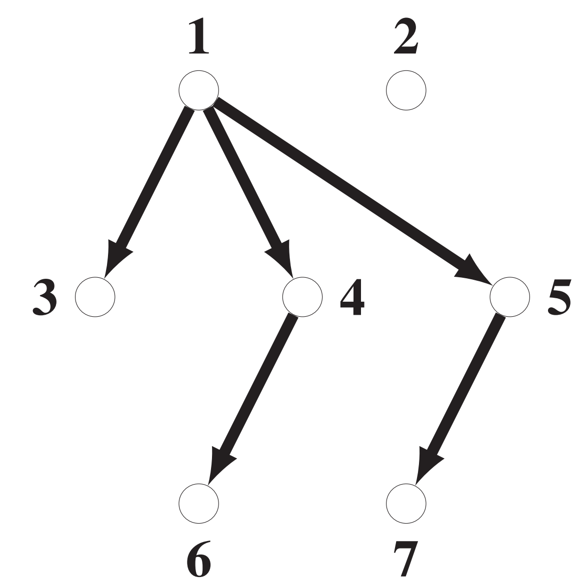
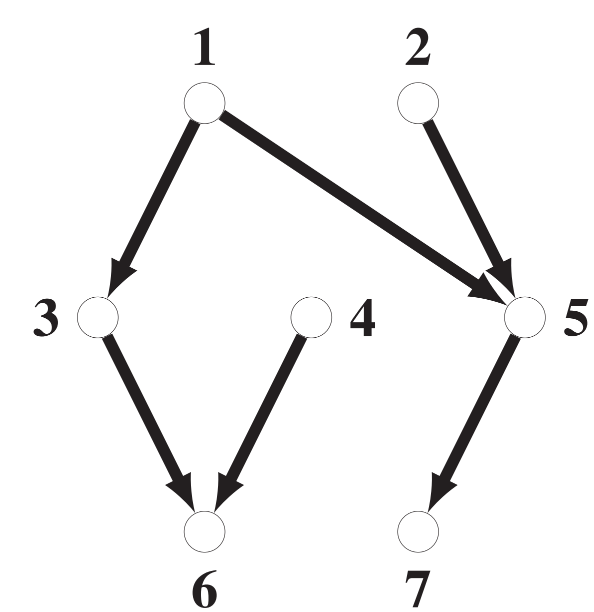


A branching

Theorem: Finding an optimal *polytree* is NP-hard [Dasgupta 1999]



A polytree

Beyond Branchings

Theorem: An optimal *branching* can be found in polynomial time.
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k-branching = polytree such that after deleting certain k arcs, every node has at most one parent.

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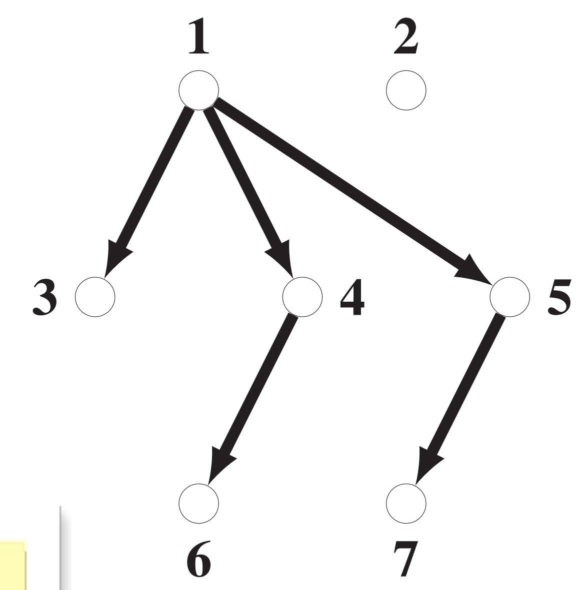

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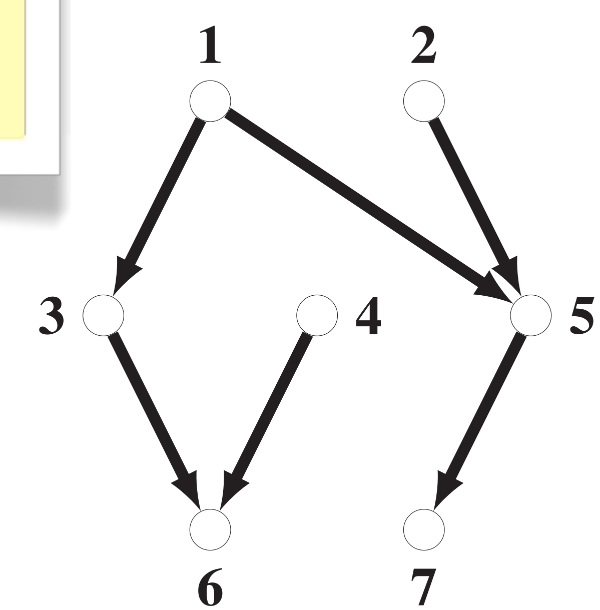

A polytree

XP-Result

Theorem: finding an optimal k-branching is polynomial for every constant k.

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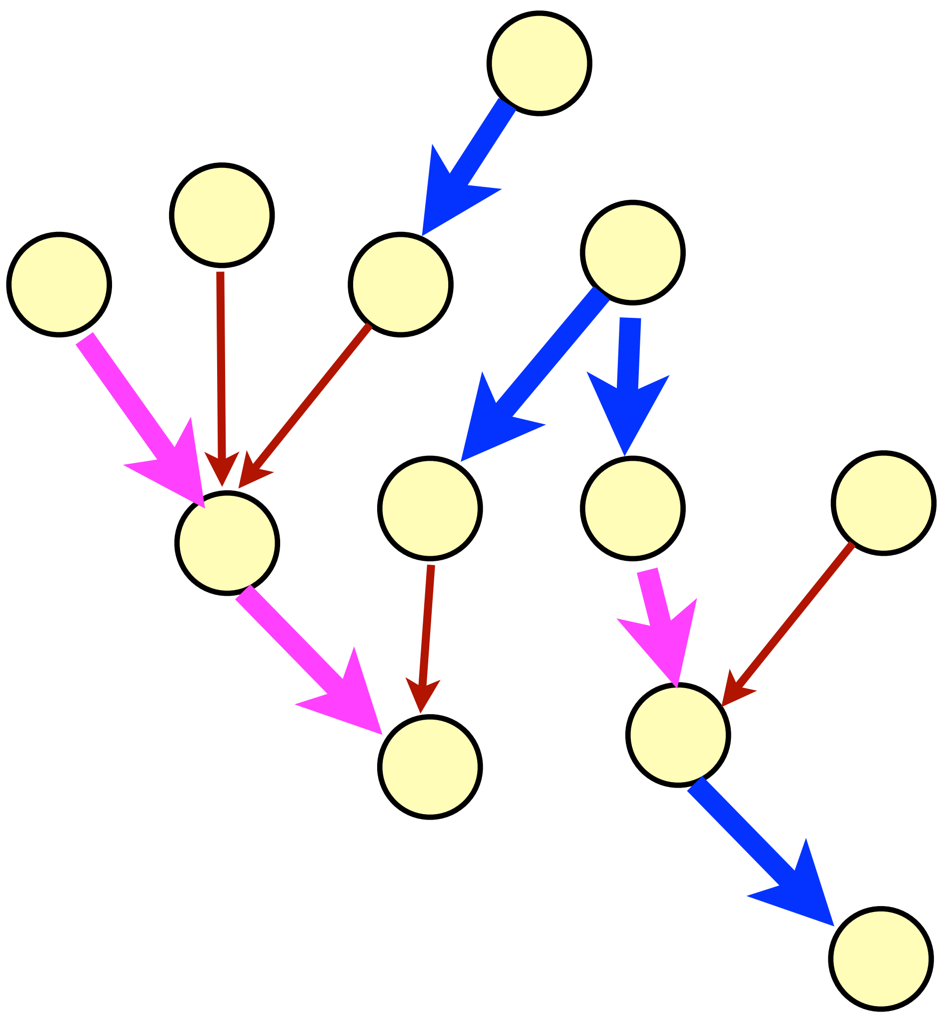
Approach:
(1) guess the deleted arcs
(2) solve the induced problem for branchings
turns out to be quite tricky!

A k-branching (k=4)



+ + = D *k-branching*

= X *deletion set*

= X‘ *co-set*

= R *rest*

+ = R∪X’=D-X polytree with in-deg ≤ 1

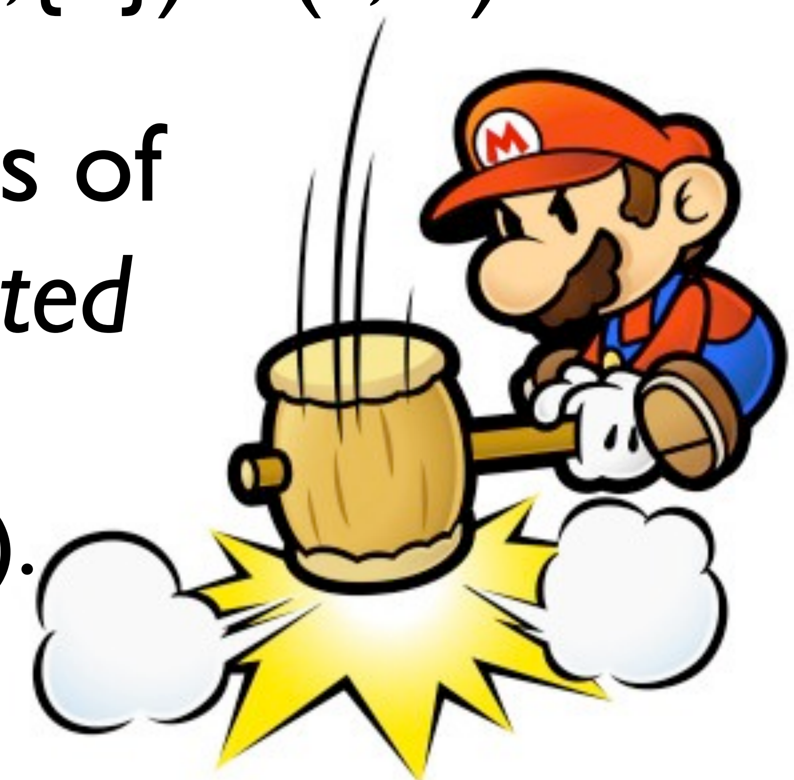
|X|≤k and |X’|≤k. Hence for constant k we can try all X and X‘ in polynomial time. For each choice of X∪X’ we compute the best set R such that R∪X’ is a polytree with in-deg ≤ 1.

Matroid Approach

- Let X, X' be two disjoint sets of arcs.
- We define define two matroids over N×N.
- The **in-degree matroid** where a set R is independent iff $R \cap (X \cup X') = \varnothing$ and R has indegree ≤ 1.
- The **acyclicity matroid** where a set R is independent iff $R \cup X \cup X'$ has no undirected cycles.
- *Lemma: D is a k-branching iff D-X is independent in both matroids.*

Matroid Intersection

- Hence, for each guessed set X we need to find an optimal set D that is independent in both matroids.
- Optimality can be expressed by considering weighted matroids: $w(u,v)= f(v,\{u\})-f(v,\emptyset)$.
- Solution can be found by means of a poly time algorithm for *weighted matroid intersection* (Brezovec, Cornuejols, Glover 1986).



FPT?

- We don’t know whether the k-branching problem is FPT.
- We have FPT algorithms for special cases whenever the guess-phase is FPT.
- For instance: *the arcs in* $X \cup X'$ *form an in-tree and each node has a bounded number of potential parent sets.*
- BN structure learning remains NP-hard under this restriction.

A slight generalization is W[1]-hard

Define a *k-node branching* as a polytree that becomes a branching by deletion of k *nodes*.

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Proof: reduction from multicolored clique.

Conclusion

- BN Network Structure Learning
- important and notoriously difficult
- parameterized complexity approach:
    - *treewidth of super structure*
    - *parameterized local search*
    - *k-branchings and k-node branchings*
- Other parameters?