

# Advances in Combinatorial Optimization Tasks over Graphical Models

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Mateescu and Lars  
Otten***



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# Outline

- Graphical models: the primary reasoning principles
    - OR Search Trees
    - AND/OR Search Trees
    - AND/OR Branch-and-Bound and Best-First Search
    - Lower Bounding Heuristics
    - Experiments
  - More recent work
- 2004-2009
- 2010-now



# Example Constraint Networks

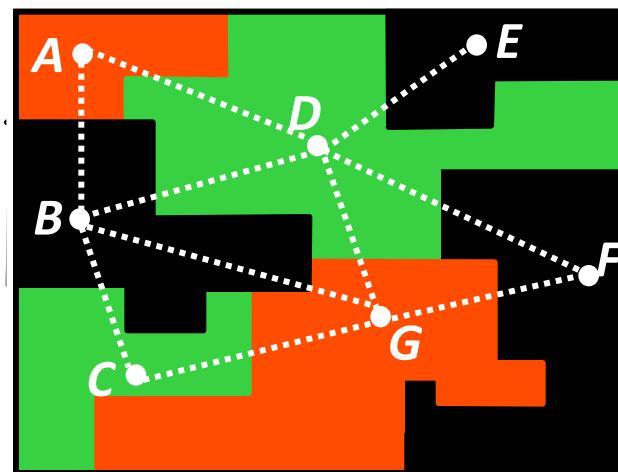
## *Map coloring*

**Variables:** countries (A B C etc.)

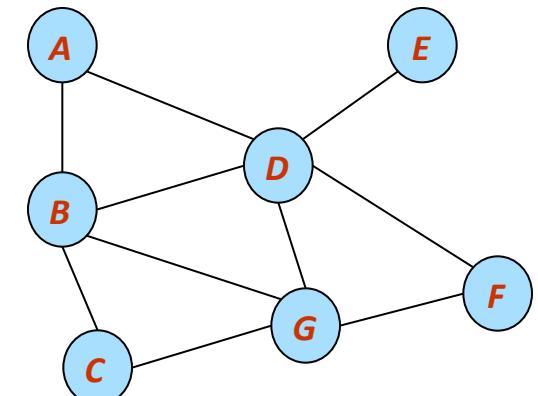
**Values:** colors (red green blue)

**Constraints:**  $A \neq B, A \neq D, D \neq E, \dots$

A	B
red	green
red	yellow
green	red
green	yellow
yellow	green
yellow	red



## *Constraint graph*



**Queries:** Find one solution, all solutions, counting

# Constraint Optimization Problems

## for Graphical Models

A *finite COP* is a triple  $R = \langle X, D, F \rangle$  where:

$X = \{X_1, \dots, X_n\}$  - variables

$D = \{D_1, \dots, D_n\}$  - domains

$F = \{f_1, \dots, f_m\}$  - cost functions

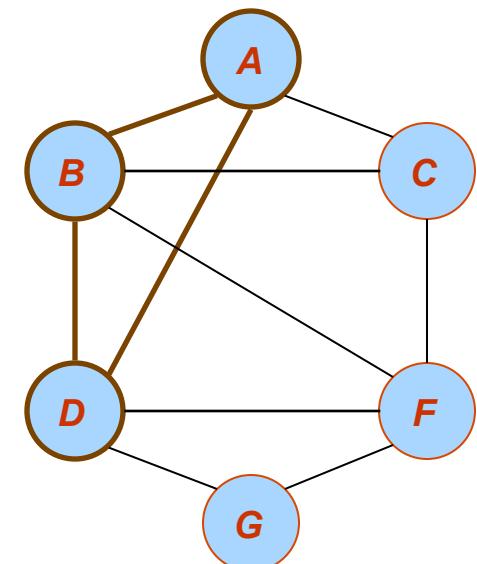
$f(A,B,D)$  has scope  $\{A,B,D\}$

A	B	D	Cost
1	2	3	3
1	3	2	2
2	1	3	$\infty$
2	3	1	0
3	1	2	5
3	2	1	0

**Primal graph =**

Variables --> nodes

Functions, Constraints -> arcs



$$F(a,b,c,d,f,g) = f_1(a,b,d) + f_2(d,f,g) + f_3(b,c,f)$$

Global Cost Function

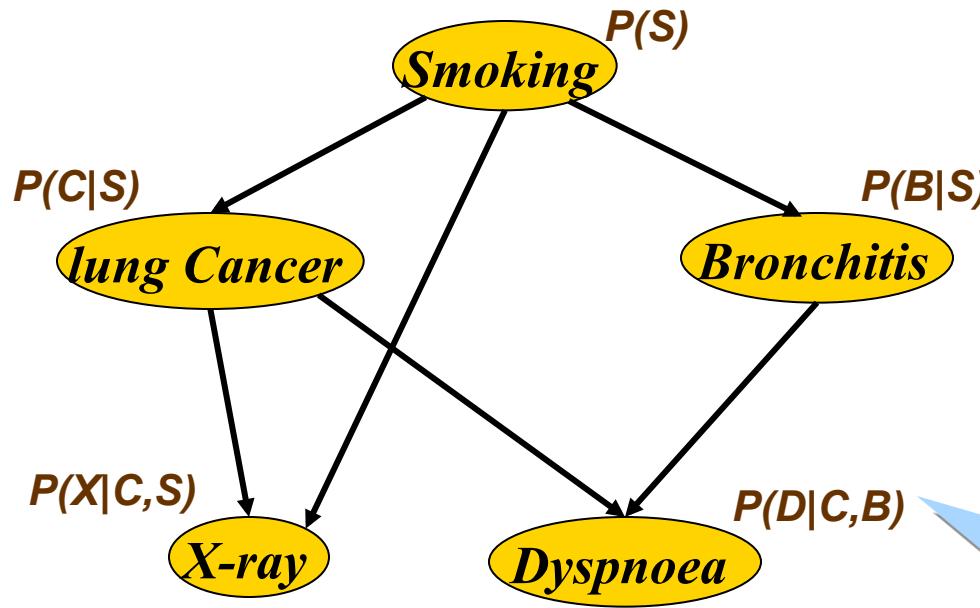
$$F(X) = \sum_{i=1}^m f_i(X)$$

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# Bayesian Networks

## The MAP/MPE Problem over Bayesian Networks



$$BN = (G, \Theta)$$

CPD:

C	B	P(D C,B)	
0	0	0.1	0.9
0	1	0.7	0.3
1	0	0.8	0.2
1	1	0.9	0.1

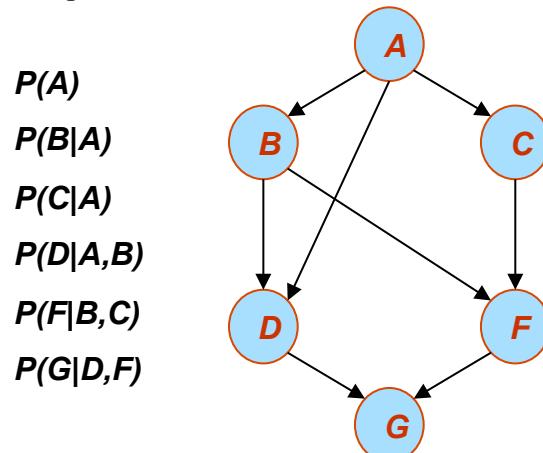
$$P(S, C, B, X, D) = P(S) P(C|S) P(B|S) P(X|C,S) P(D|C,B)$$

**Posterior marginals, Most probable tuple (MPE)**

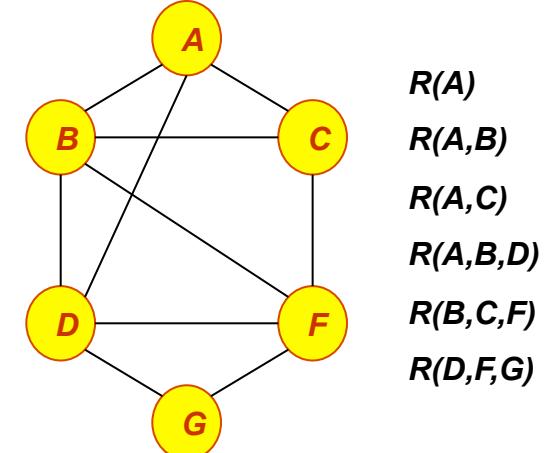
- MPE/MAP= *find argmax P(S) · P(C|S) · P(B|S) · P(X|C,S) · P(D|C,B) =?*



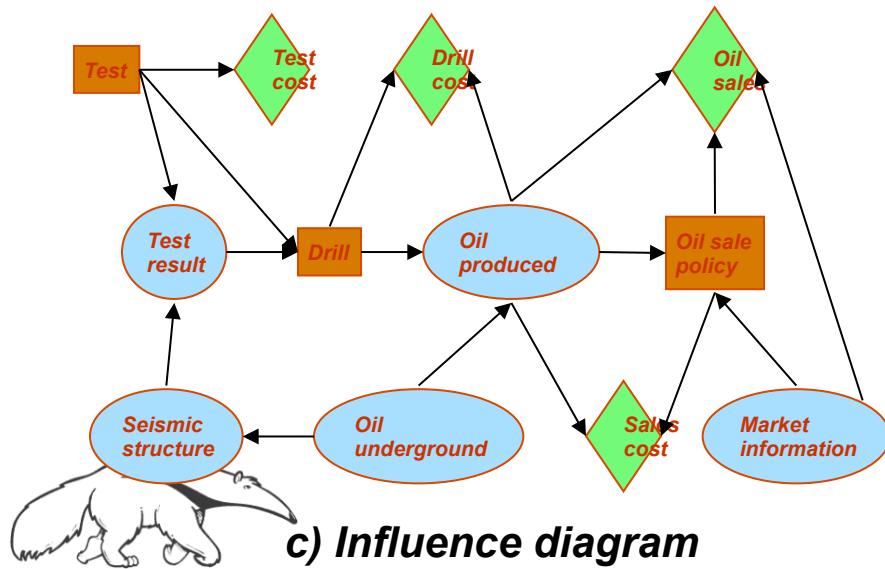
# Graphical Models



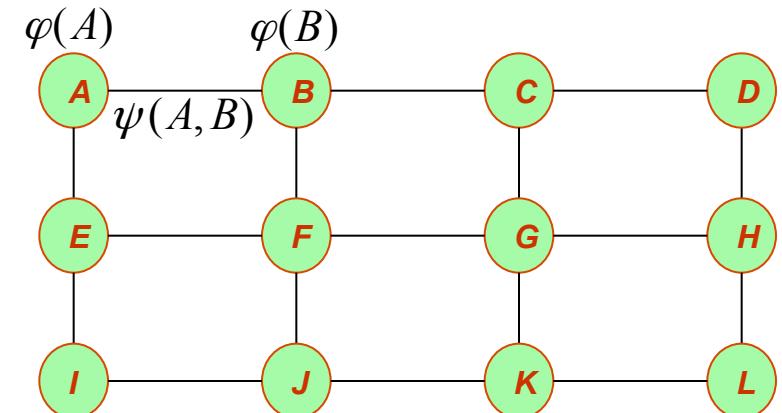
a) Belief network



b) Constraint network



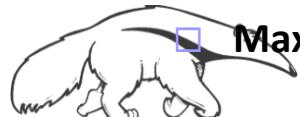
c) Influence diagram



d) Markov network

# Graphical Models

- A graphical model  $(X, D, F)$ :
  - $X = \{X_1, \dots, X_n\}$  variables
  - $D = \{D_1, \dots, D_n\}$  domains
  - $F = \{f_1, \dots, f_r\}$  functions  
(constraints, CPTs, CNFs ...)
- Operators:
  - combination
  - elimination (projection)
- Tasks:
  - Belief updating:  $\sum_{x-y} \prod_j P_i$
  - MPE:  $\max_x \prod_j P_j$
  - CSP:  $\prod_{x-y} C_j$
  - Max-CSP:  $\min_X \sum_j F_j$

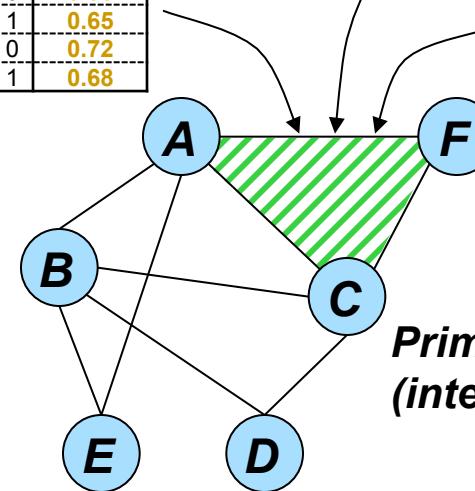


**Conditional Probability Table (CPT)**

A	C	F	$P(F A,C)$
0	0	0	0.14
0	0	1	0.96
0	1	0	0.40
0	1	1	0.60
1	0	0	0.35
1	0	1	0.65
1	1	0	0.72
1	1	1	0.68

**Relation**

A	C	F
red	green	blue
blue	red	red
blue	blue	green
green	red	blue



**Primal graph  
(interaction graph)**

- **All these tasks are NP-hard**
  - **exploit problem structure**
  - **identify special cases**
  - **approximate**

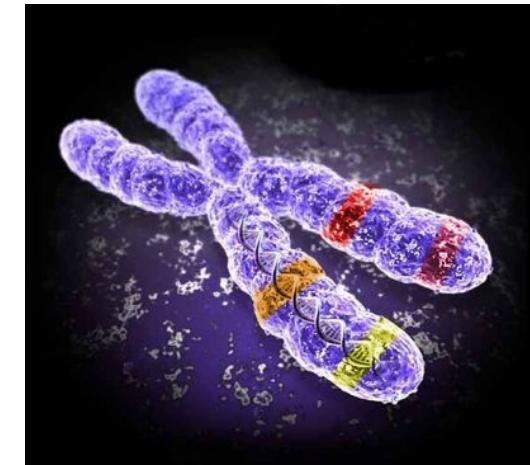
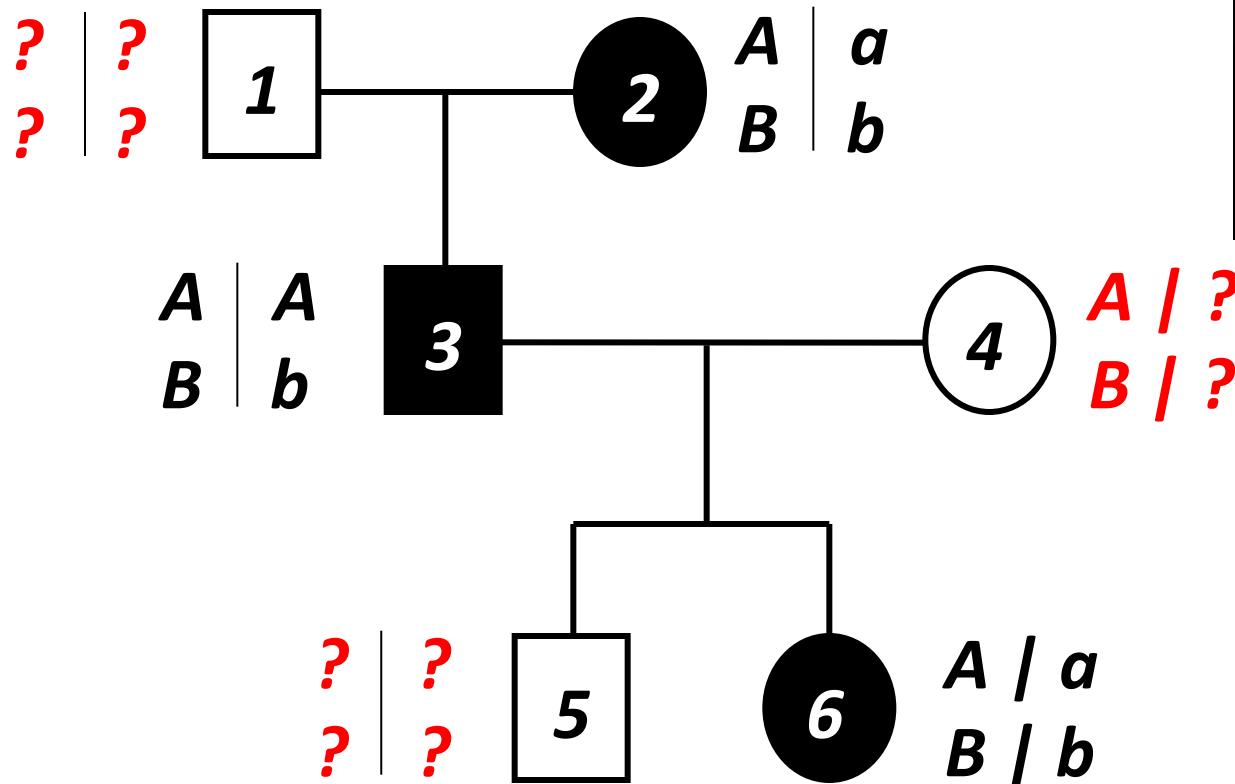
# Types of Constraint Optimization

- Valued CSPs, Weighted CSPs, Max-CSPs, Max-SAT
- Most Probable Explanation (MPE/MAP)
- Linear Integer Programs

- **Examples:**
  - Problems translated from planning
  - Unit scheduling maintenance
  - Combinatorial auctions
  - Maximum-likelihood haplotypes in linkage



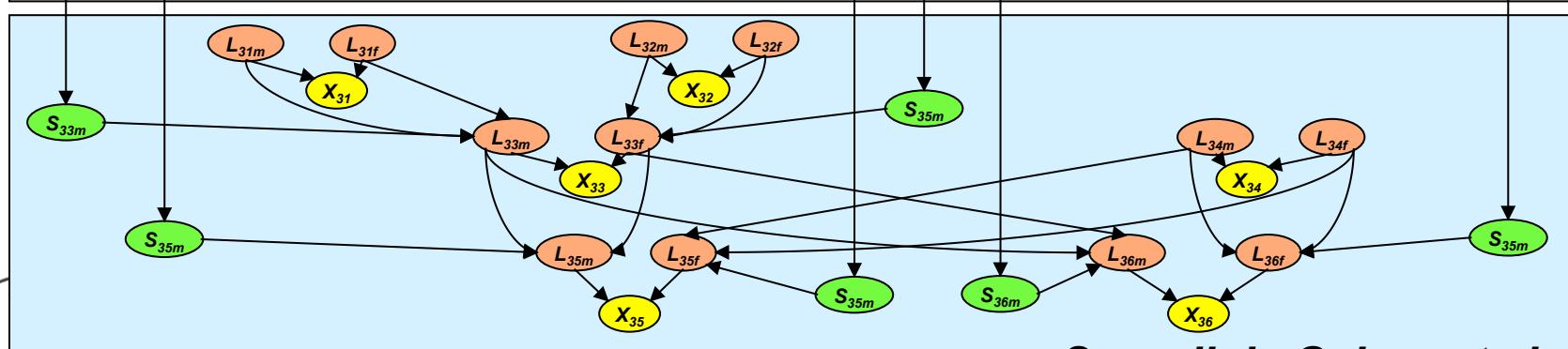
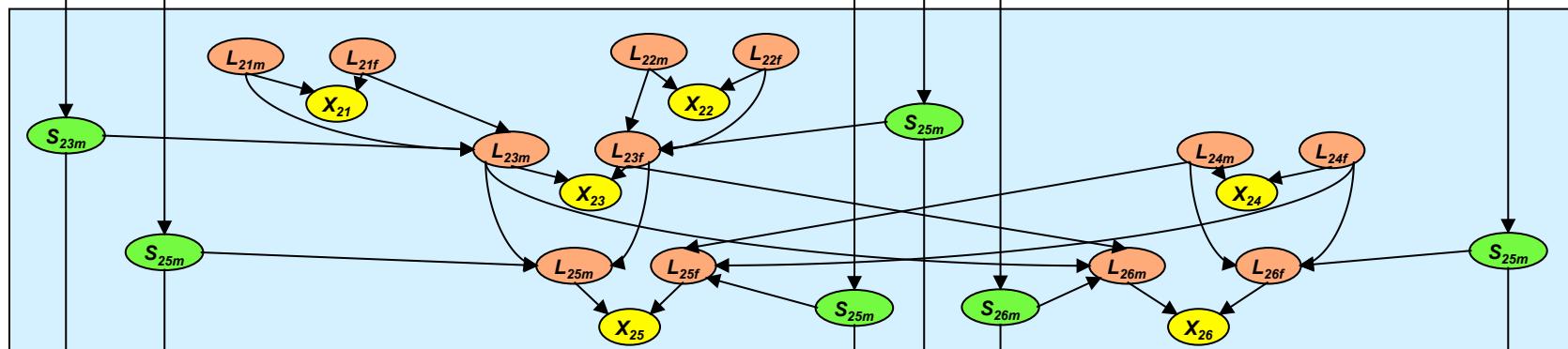
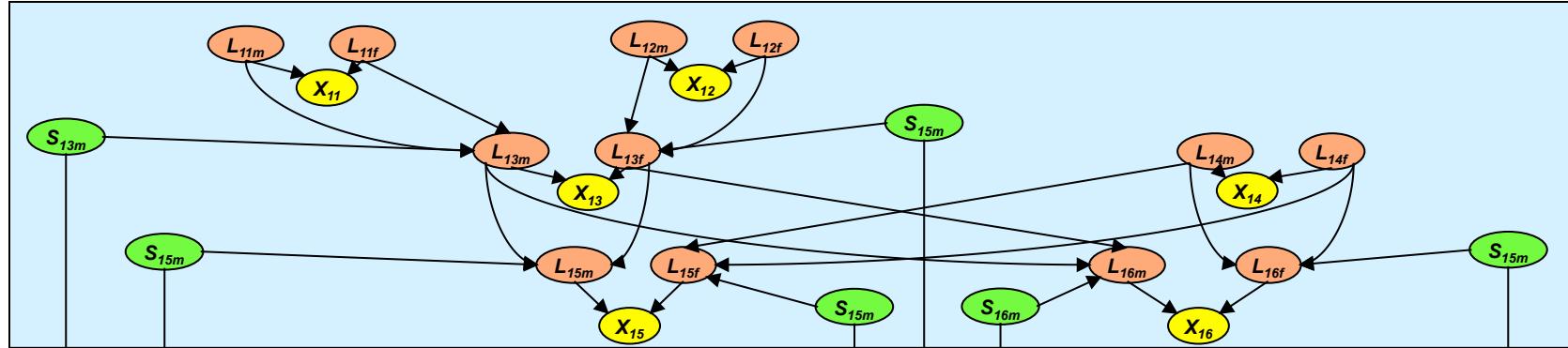
# Linkage Analysis



- 6 individuals
- Haplotype: {2, 3}
- Genotype: {6}
- Unknown



# Pedigree: 6 people, 3 markers



**Superlink, Geiger et.al**



# Solution Techniques, State of the art

## AND/OR search

*Time:*  $\exp(\text{treewidth} * \log n)$

*Space:* linear

*Space:*  $\exp(\text{treewidth})$

*Time:*  $\exp(\text{treewidth})$

### Complete

DFS search

Branch-and-Bound

A\*

*Time:*  $\exp(\text{treewidth})$

*Space:*  $\exp(\text{treewidth})$

## Search (Conditioning)

*Time:*  $\exp(n)$

*Space:* linear

*Time:*  $\exp(\text{pathwidth})$

*Space:*  $\exp(\text{pathwidth})$

### Incomplete

Simulated Annealing

Gradient Descent

Stochastic Local Search

### Hybrids

### Complete

Adaptive Consistency

Tree Clustering

Variable Elimination

Resolution

### Incomplete

Belief-propagation

Unit Resolution

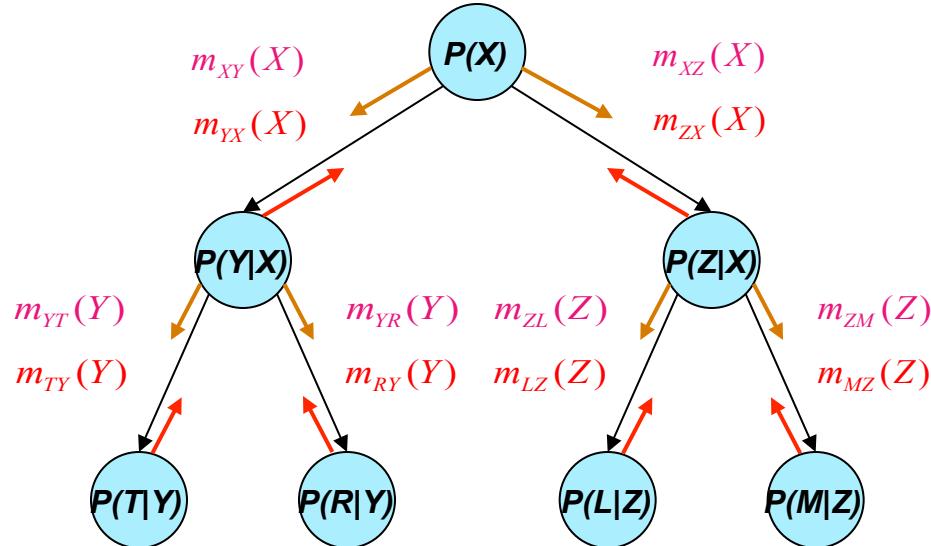
Mini-bucket(i)

## Inference (Elimination)



# Tree-solving is Easy

*Belief updating  
(sum-prod)*



*CSP – consistency  
(projection-join)*

*Dynamic Programming*

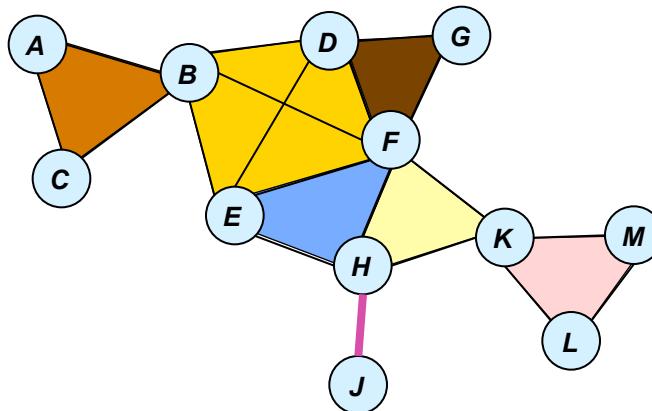
*MPE (max-prod)*

*#CSP (sum-prod)*

*Trees are processed in linear time and memory  
Also Acyclic graphical models*  
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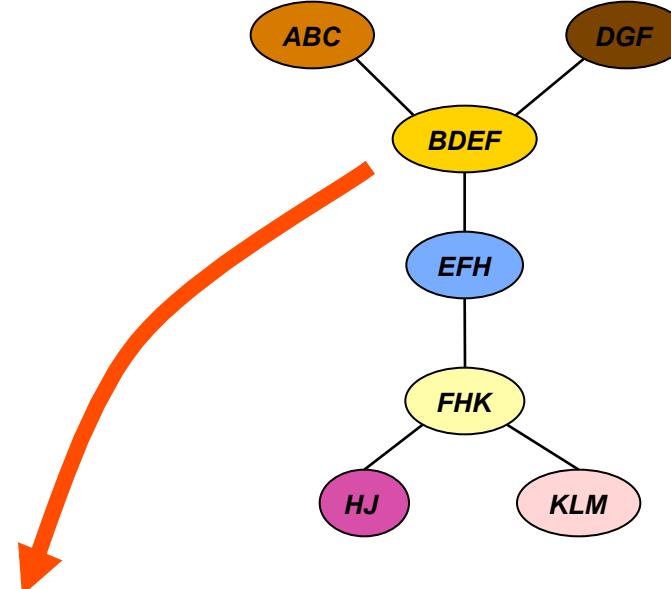
# Inference and Treewidth



**Inference algorithm:**

**Time:**  $\exp(\text{tree-width}+1)$

**Space:**  $\exp(\text{separator-width})$



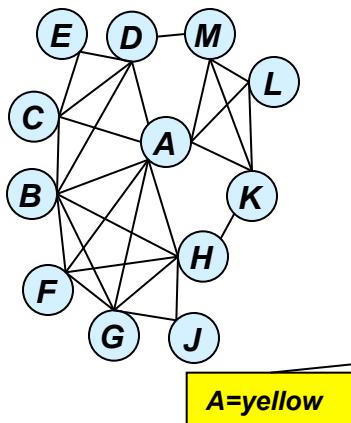
$$\text{treewidth} = 4 - 1 = 3$$

$$\text{treewidth} = (\text{maximum cluster size}) - 1$$

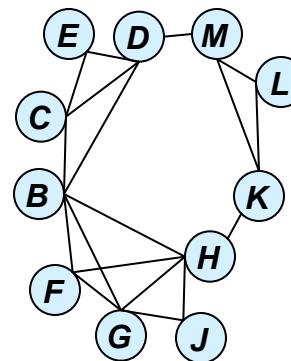
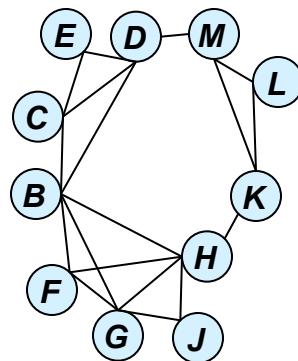
$$\text{Separator-width} = 2$$

# Search over the Cutset

**Graph  
Coloring  
problem**

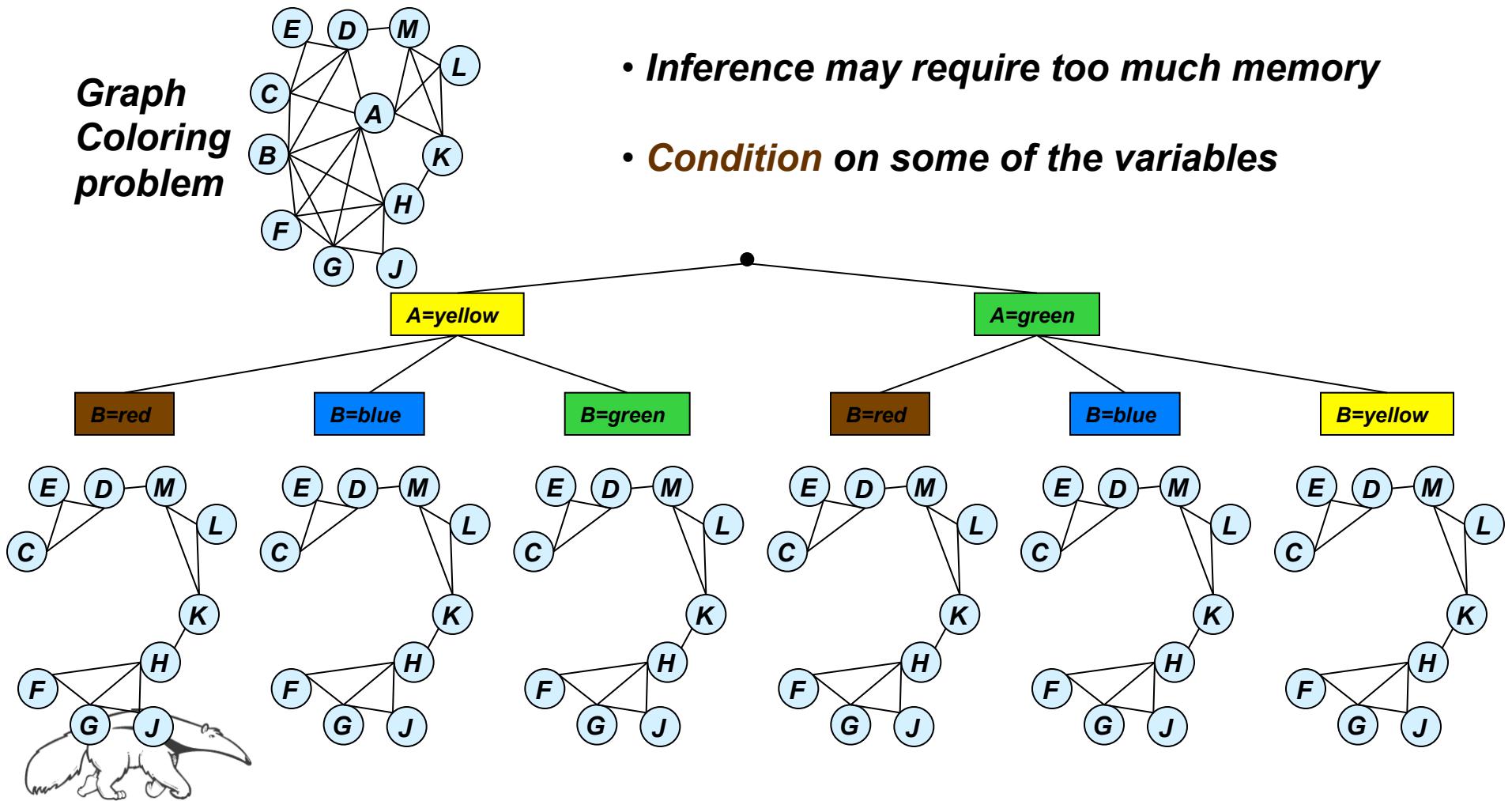


- *Inference may require too much memory*
- *Condition (guessing) on some of the variables*



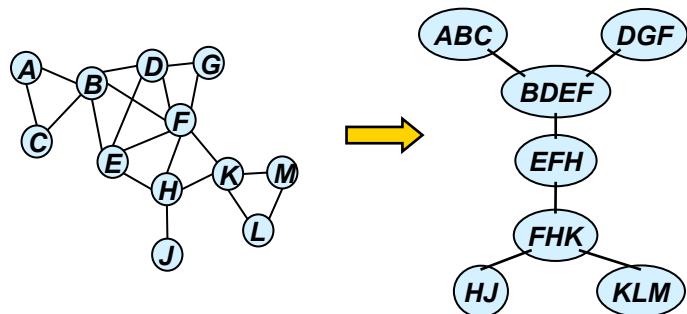
# Search over the Cutset (cont)

**Graph  
Coloring  
problem**



# Inference vs. Conditioning

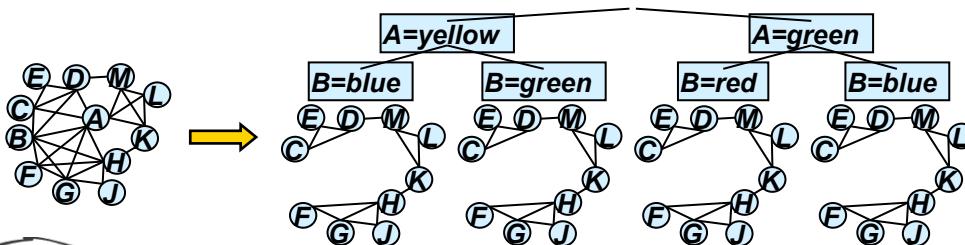
- By Inference (thinking)



*Exponential in treewidth  
Time and space*

- By Conditioning (guessing)

•



*Exponential in cycle-cutset  
Time. linear space*



# Inference for Optimization: Bucket Elimination

*Algorithm BE-mpe (Dechter 1996, Bertele and Brioschi, 1977)*

$$MPE = \max_{a,e,d,c,b} P(a)P(c|a)P(b|a)P(d|a,b)P(e|b,c)$$

*bucket B:*

$$\max_X \prod \underbrace{P(b|a) \quad P(d|b,a) \quad P(e|b,c)}_{}$$

*bucket C:*

$$P(c|a) \quad h^B(a, d, c, e)$$

*bucket D:*

$$h^c(a, d, e)$$

*bucket E:*

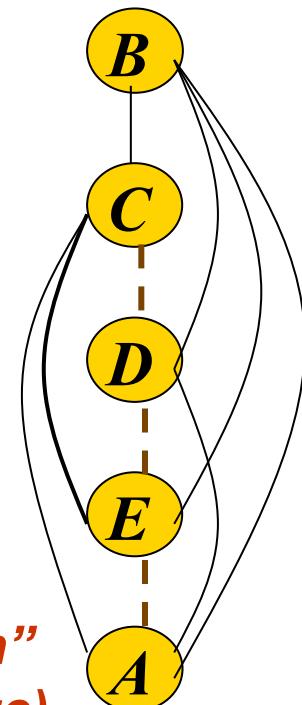
$$e=0 \quad h^D(a, e)$$

*bucket A:*

$$P(a) \quad h^E(a)$$

*OPT*

$W^*=4$   
"induced width"  
(max clique size)



# Generating the MPE-tuple

$$5. \ b' = \arg \max P(b | a') \times \\ \times P(d' | b, a') \times P(e' | b, c')$$

$$4. \ c' = \arg \max P(c | a') \times \\ \times h^B(a', d', c, e')$$

$$3. \ d' = \arg \max_d h^c(a', d, e')$$

$$2. \ e' = 0$$

$$1. \ a' = \arg \max_a P(a) \cdot h^E(a)$$

	$B:$	$P(b a)$	$P(d b,a)$	$P(e b,c)$
	$C:$	$P(c a)$	$h^B(a, d, c, e)$	
	$D:$		$h^c(a, d, e)$	
	$E:$	$e=0$		$h^D(a, e)$
	$A:$	$P(a)$		$h^E(a)$

*Return (a', b', c', d', e')*



# Solution methods

- Solving tree is easy
- Inference: move to trees by clustering
  - (dynamic programming, variable elimination, junction trees)
  - Exploit structure well.
- Search: move to trees by conditioning.
  - Can also exploit structure well.

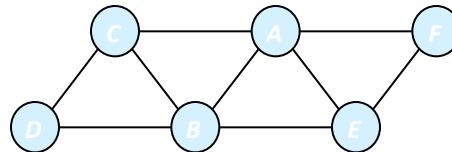


# Outline

- Graphical Models: reasoning principles
- OR Search Trees
- AND/OR Search Spaces for GM
- AND/OR Branch-and-Bound and Best-First Search
- Lower Bounding Heuristics
- Experimental evaluation
- Current work

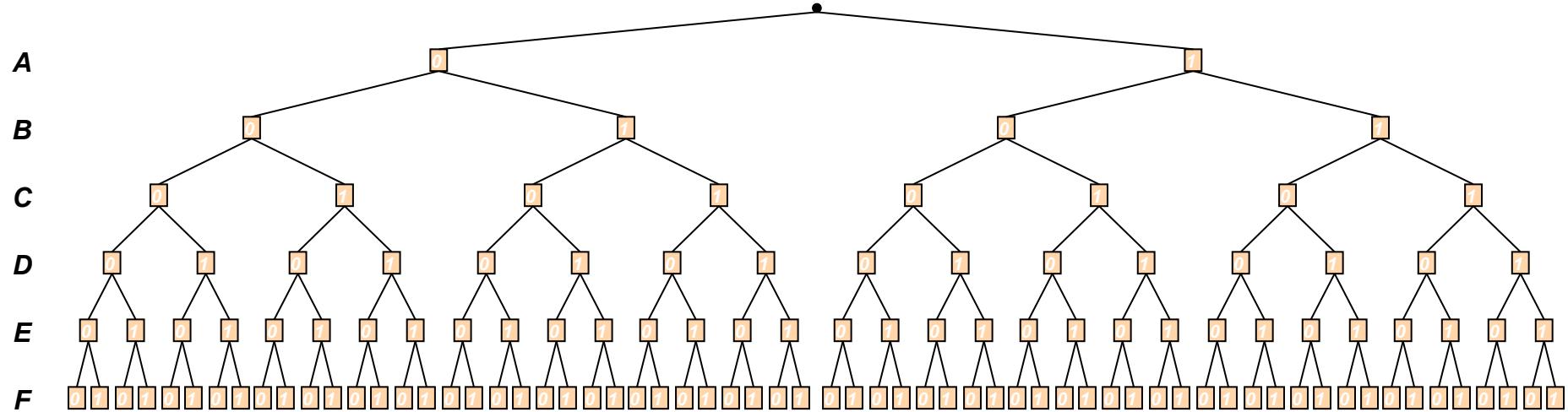


# The Search Space

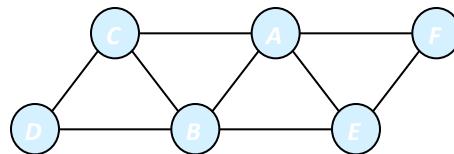


A	B	f <sub>1</sub>	A	C	f <sub>2</sub>	A	E	f <sub>3</sub>	A	F	f <sub>4</sub>	B	C	f <sub>5</sub>	B	D	f <sub>6</sub>	B	E	f <sub>7</sub>	C	D	f <sub>8</sub>	E	F	f <sub>9</sub>				
0	0	2	0	0	3	0	0	0	0	0	2	0	0	0	0	0	4	0	0	3	0	0	1	0	0	1				
0	1	0	0	1	0	0	1	3	0	1	0	0	1	1	0	1	1	2	1	0	1	2	0	1	4	1	0	0		
1	0	1	1	0	0	1	0	2	1	0	0	2	1	0	2	1	1	4	1	1	0	1	0	1	0	1	0	0	1	
1	1	4	1	1	1	1	1	0	1	1	2	0	1	1	4	1	1	0	1	1	0	1	1	0	1	1	0	1	1	2

$$f(\mathbf{x}) = \min_X \sum_{i=1}^9 f_i(\mathbf{x})$$

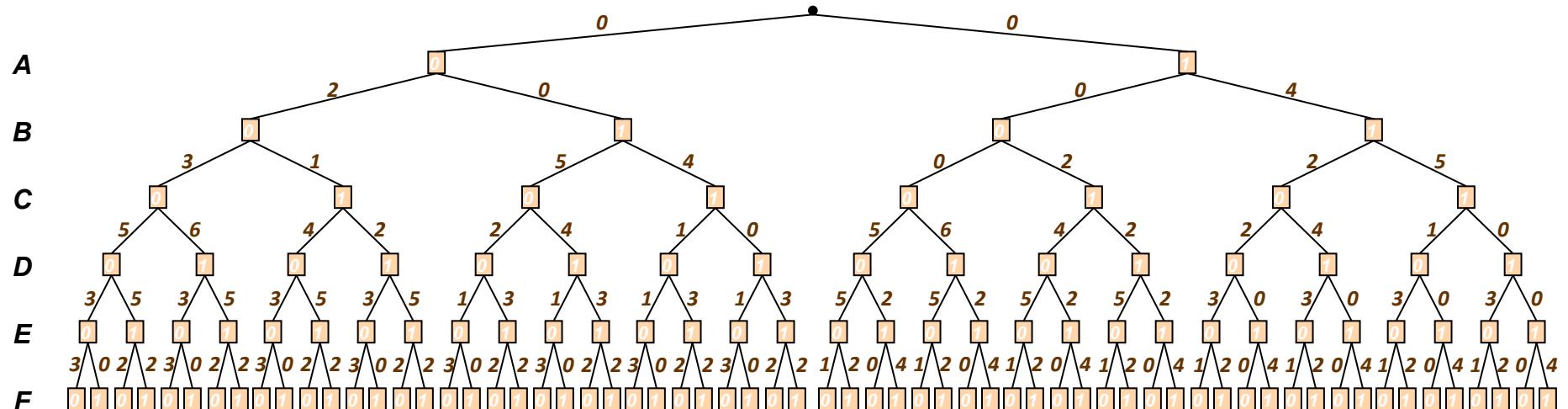


# The Search Space



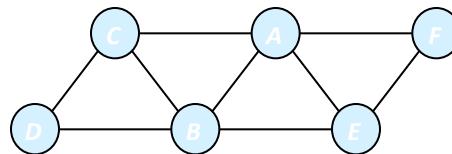
A	B	$f_1$	A	C	$f_2$	A	E	$f_3$	A	F	$f_4$	B	C	$f_5$	B	D	$f_6$	B	E	$f_7$	C	D	$f_8$	E	F	$f_9$			
0	0	2	0	0	3	0	0	0	0	0	2	0	0	0	0	0	4	0	0	3	0	0	1	0	0	1			
0	1	0	0	1	0	0	1	3	0	1	0	0	1	1	0	1	2	1	0	1	2	0	1	4	1	0	0		
1	0	1	1	0	0	1	0	2	1	0	0	2	1	0	2	1	1	4	1	1	0	1	0	1	0	1	0	0	
1	1	4	1	1	1	1	1	0	1	1	2	1	1	4	1	1	0	1	1	0	1	1	0	1	1	0	1	1	2

$$f(\mathbf{X}) = \min_X \sum_{i=1}^9 f_i(\mathbf{X})$$



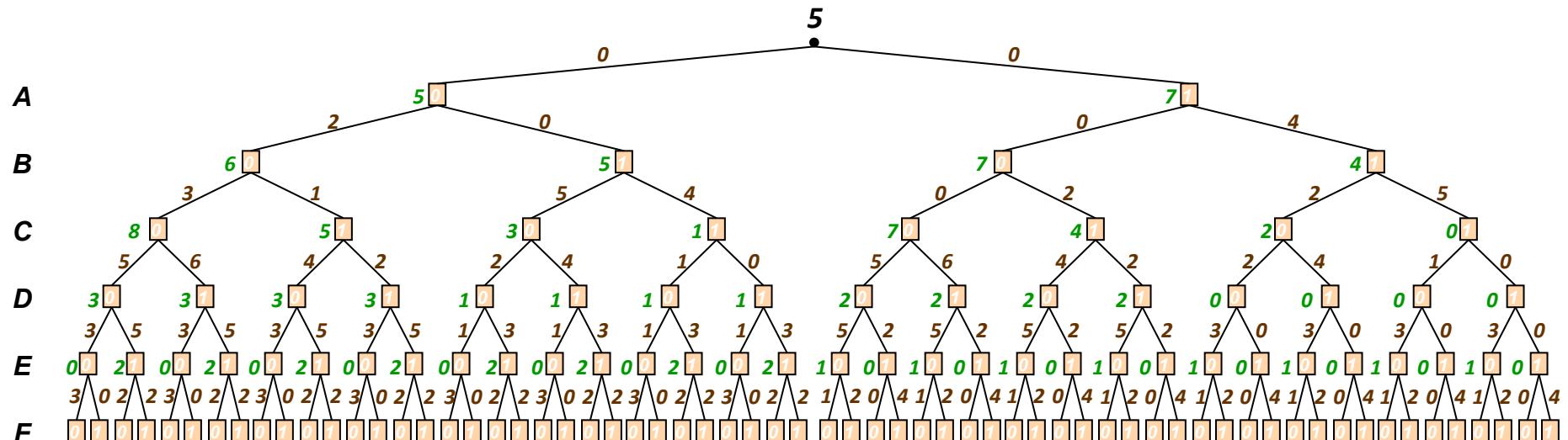
*are calculated based on cost components*

# The Search Space



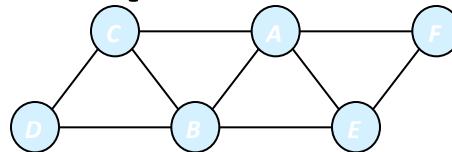
A	B	f <sub>1</sub>	A	C	f <sub>2</sub>	A	E	f <sub>3</sub>	A	F	f <sub>4</sub>	B	C	f <sub>5</sub>	B	D	f <sub>6</sub>	B	E	f <sub>7</sub>	C	D	f <sub>8</sub>	E	F	f <sub>9</sub>			
0	0	2	0	0	3	0	0	0	0	0	2	0	0	0	0	0	4	0	0	3	0	0	1	0	0	1			
0	1	0	0	1	0	0	1	3	0	1	0	0	1	1	0	1	2	1	0	1	2	0	1	4	1	0	0		
1	0	1	1	0	0	1	0	2	1	0	0	1	0	2	1	1	4	1	1	0	1	0	1	0	1	0	0	2	
1	1	4	1	1	1	1	1	0	1	1	2	1	1	4	1	1	0	1	1	0	1	1	0	1	1	0	1	1	2

$$f(\mathbf{X}) = \min_X \sum_{i=1}^9 f_i(\mathbf{X})$$



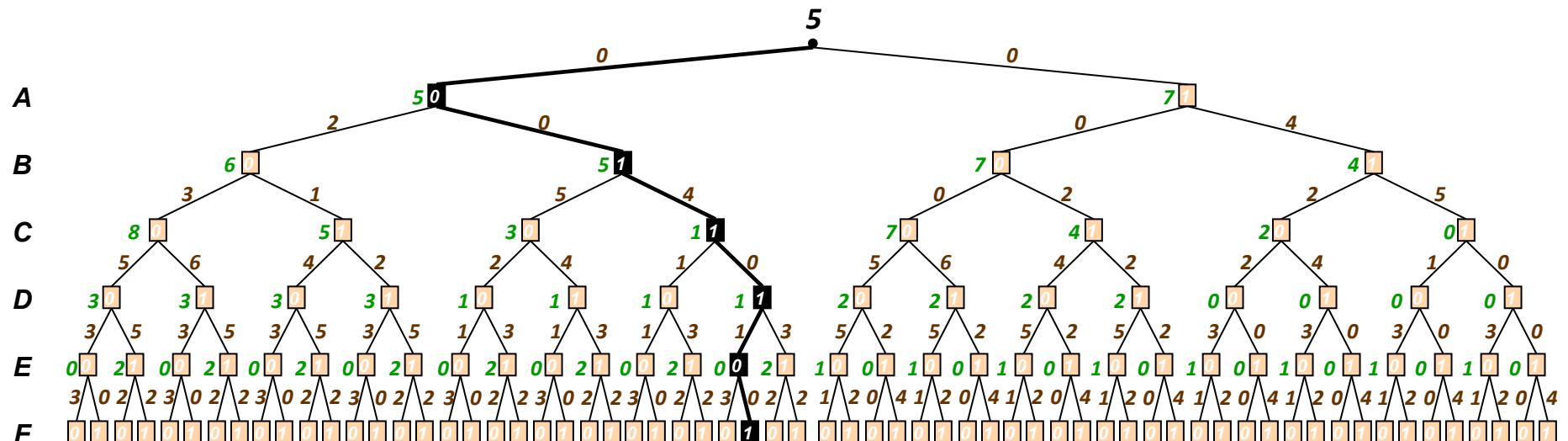
**Node value = minimal cost solution below it**

# An Optimal Solution



A	B	$f_1$	A	C	$f_2$	A	E	$f_3$	A	F	$f_4$	B	C	$f_5$	B	D	$f_6$	B	E	$f_7$	C	D	$f_8$	E	F	$f_9$			
0	0	2	0	0	3	0	0	0	0	0	2	0	0	0	0	0	4	0	0	3	0	0	1	0	0	1			
0	1	0	0	1	0	0	1	3	0	1	0	0	1	1	0	1	2	1	0	1	2	0	1	4	1	0	0		
1	0	1	1	0	0	1	0	2	1	0	0	1	0	2	1	1	4	1	1	0	1	0	1	0	1	0	0	1	
1	1	4	1	1	1	1	1	0	1	1	2	1	1	4	1	1	0	1	1	0	1	1	0	1	1	0	1	1	2

$$f(\mathbf{X}) = \min_X \sum_{i=1}^9 f_i(\mathbf{X})$$



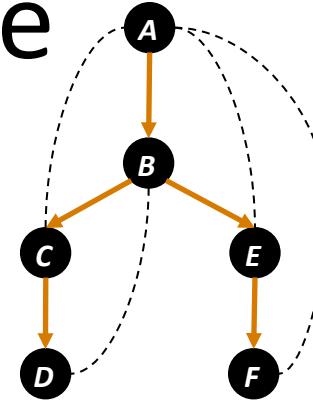
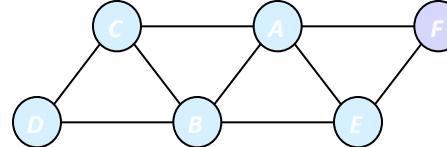
An optimal assignment is  $A=0, B=1, C=1, D=1, E=0, F=1$  with cost 5

# Outline

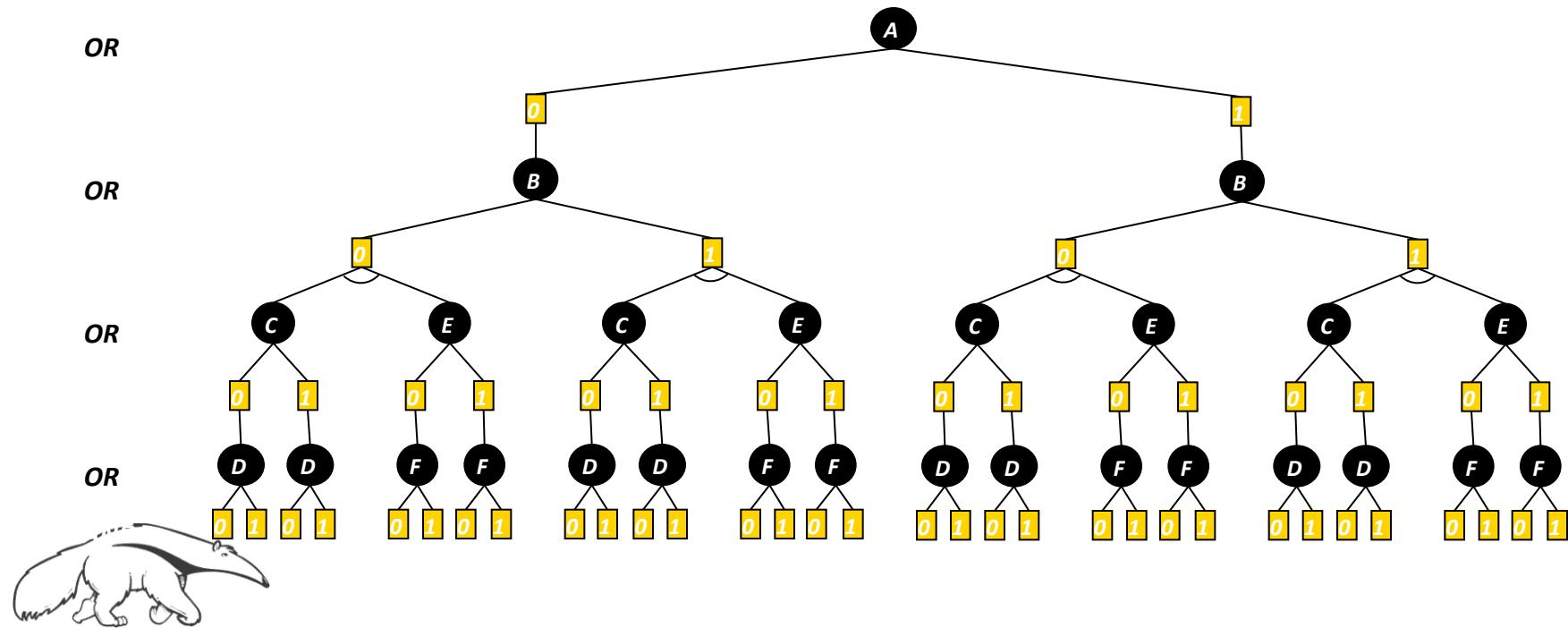
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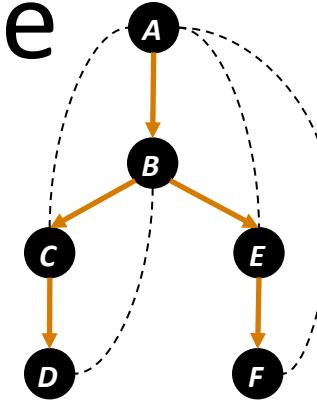
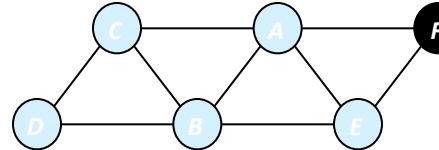
# The AND/OR Search Tree



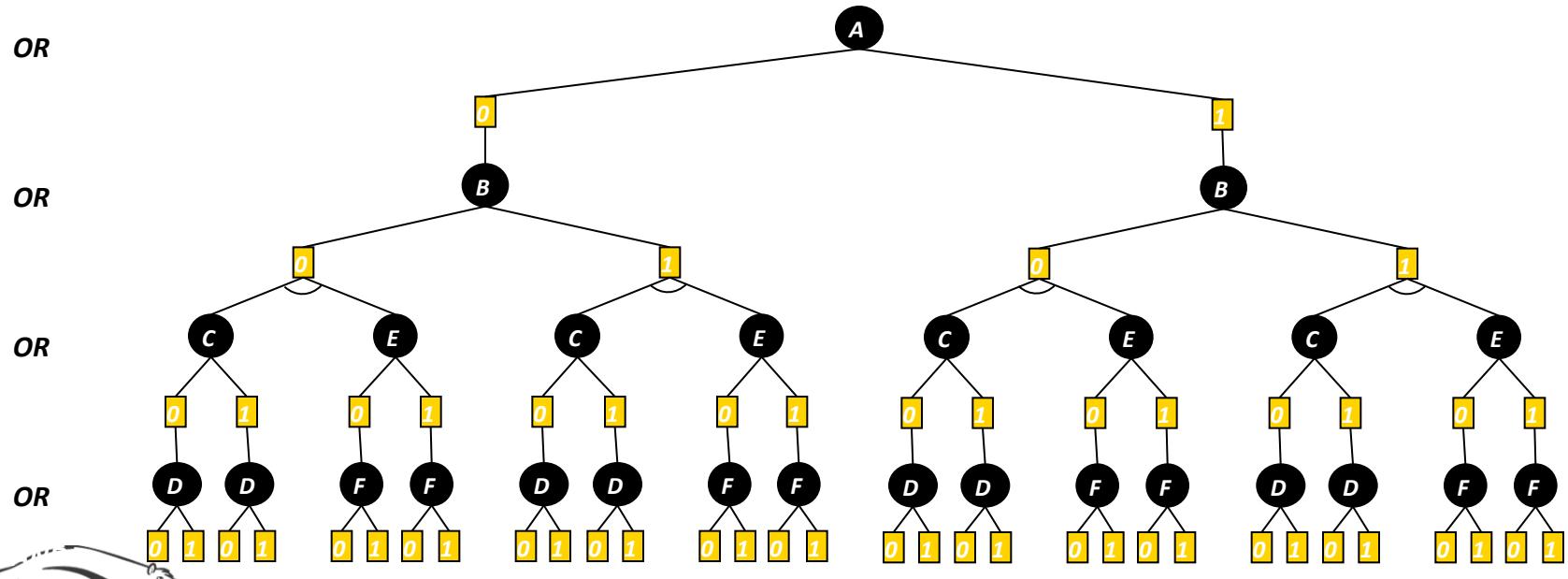
*Pseudo tree (Freuder & Quinn85)*



# The AND/OR Search Tree

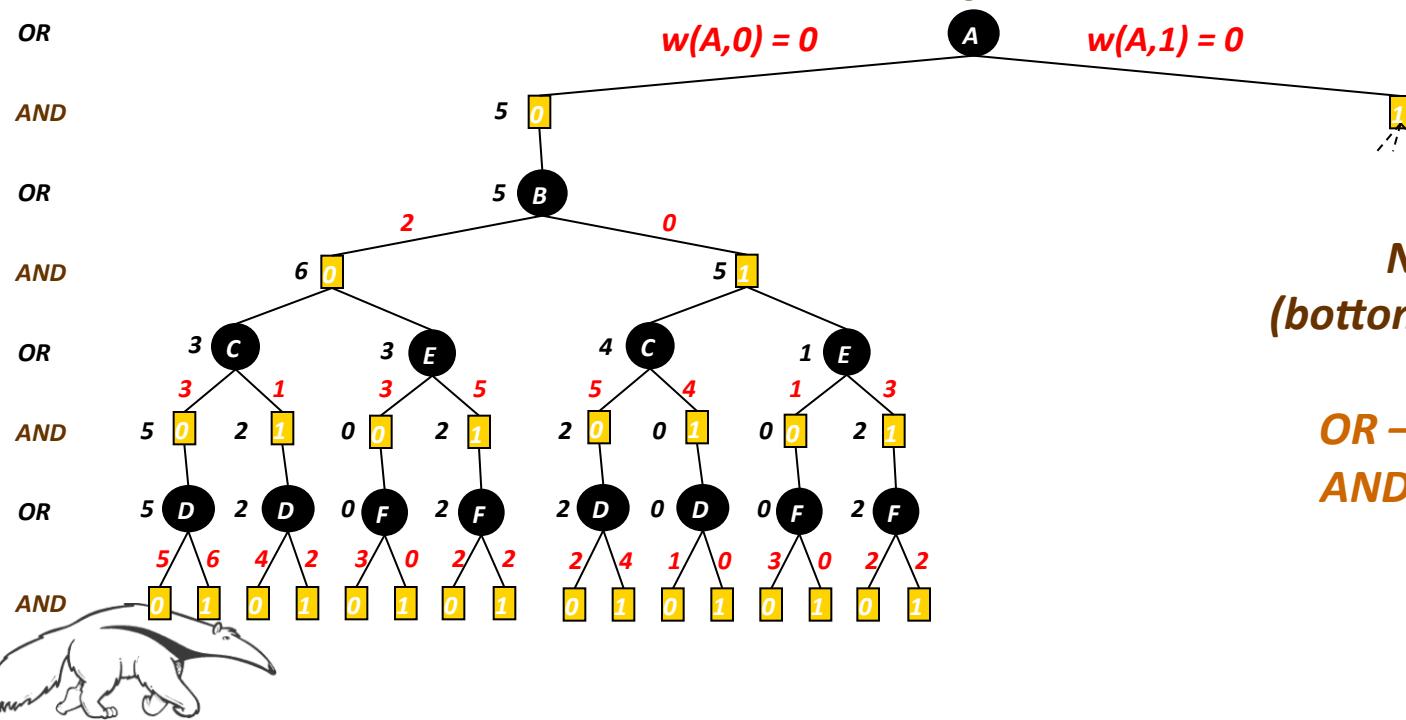
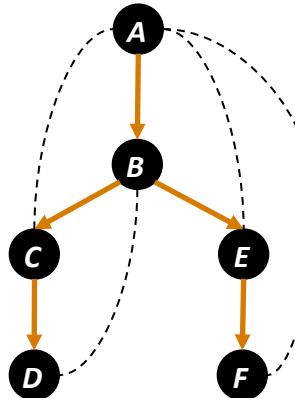
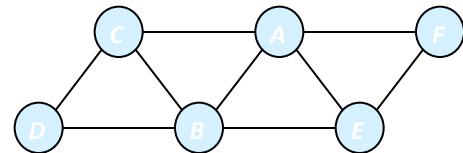


*Pseudo tree*



*A solution subtree is*

# Weighted AND/OR Search Tree



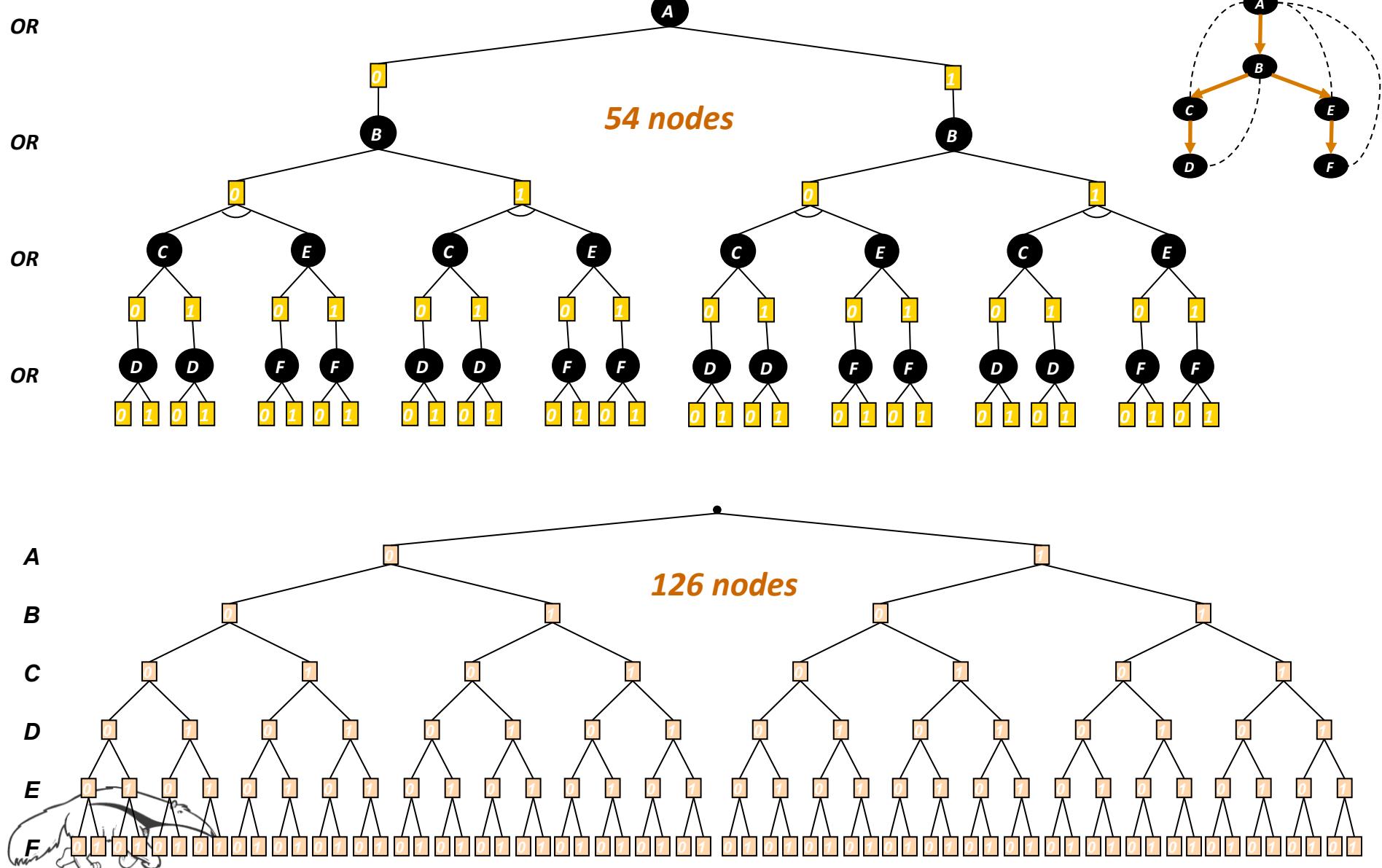
A	B	$f_1$	A	C	$f_2$	A	E	$f_3$	A	F	$f_4$	B	C	$f_5$	B	D	$f_6$	B	E	$f_7$	C	D	$f_8$	E	F	$f_9$
0	0	2	0	0	3	0	0	0	0	0	2	0	0	0	0	0	4	0	0	3	0	0	1	0	0	
0	1	0	0	1	0	0	1	3	0	1	0	0	1	1	0	1	1	2	0	1	2	0	1	4	1	0
1	0	1	1	0	0	1	0	2	1	0	0	0	1	0	2	1	0	1	1	0	1	0	1	0	1	0
1	1	4	1	1	1	1	1	0	1	1	2	1	1	4	1	1	0	1	1	0	1	1	0	1	1	2

$$f(\mathbf{X}) = \min_X \sum_{i=1}^9 f_i(\mathbf{X})$$

**Node Value**  
*(bottom-up evaluation)*

**OR – minimization**  
**AND – summation**

# AND/OR vs. OR Spaces



# AND/OR vs. OR Spaces

width	depth	OR space		AND/OR space		
		Time (sec.)	Nodes	Time (sec.)	AND nodes	OR nodes
5	10	3.15	2,097,150	0.03	<b>10,494</b>	5,247
4	9	3.13	2,097,150	0.01	<b>5,102</b>	2,551
5	10	3.12	2,097,150	0.03	<b>8,926</b>	4,463
4	10	3.12	2,097,150	0.02	<b>7,806</b>	3,903
5	13	3.11	2,097,150	0.10	<b>36,510</b>	18,255

*Random graphs with 20 nodes, 20 edges and 2 values per node*



# Complexity of AND/OR Tree Search

	AND/OR tree	OR tree
Space	$O(n)$	$O(n)$
Time	$O(n k^m)$ $O(n k^{w^*} \log n)$ (Freuder & Quinn85), (Collin, Dechter & Katz91), (Bayardo & Miranker95), (Darwiche01)	$O(k^n)$

*k* = domain size

*m* = depth of pseudo-tree

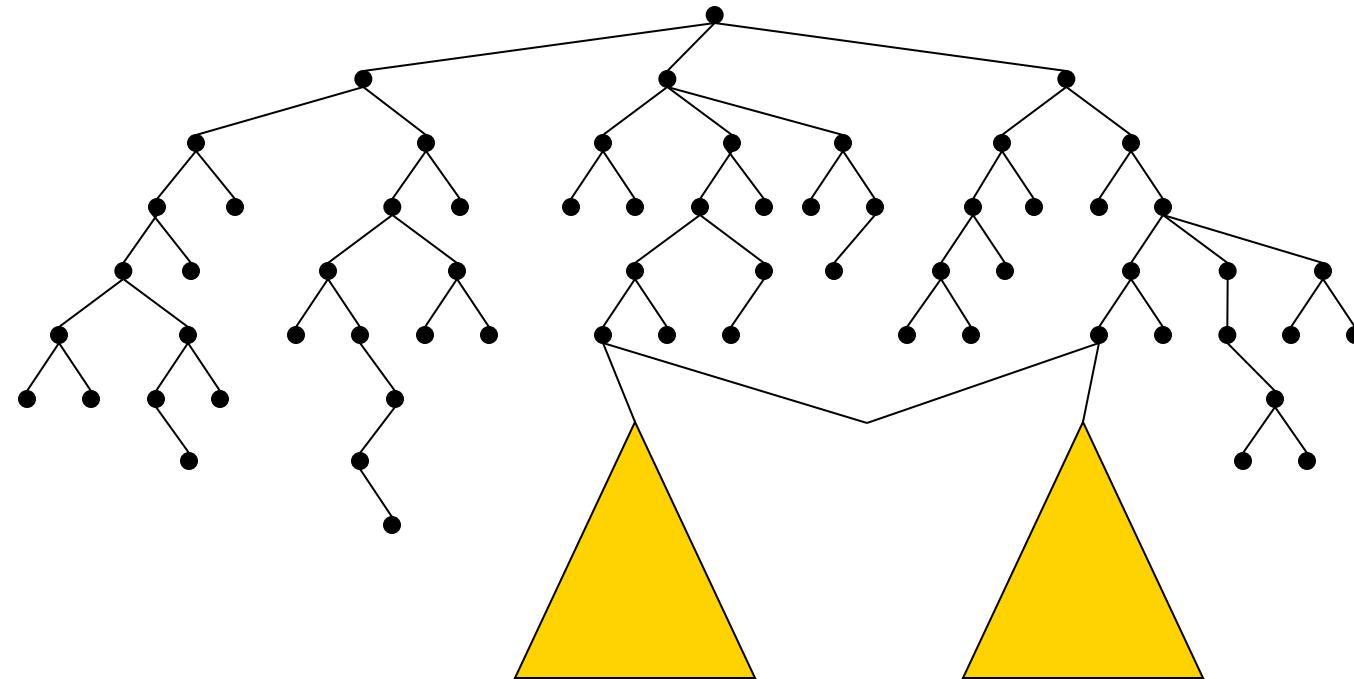
*n* = number of variables

*w\**= treewidth



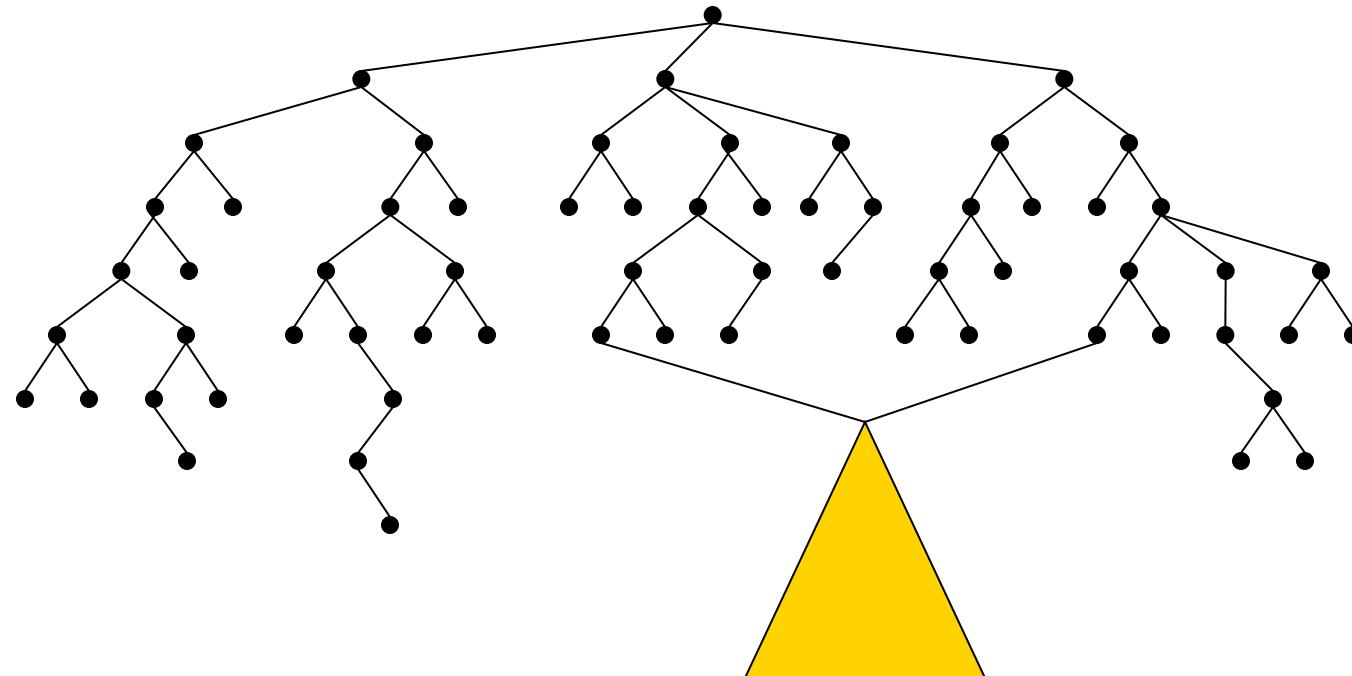
# From Search Trees to Search Graphs

- Any two nodes that root **identical** sub-trees or sub-graphs can be **merged**

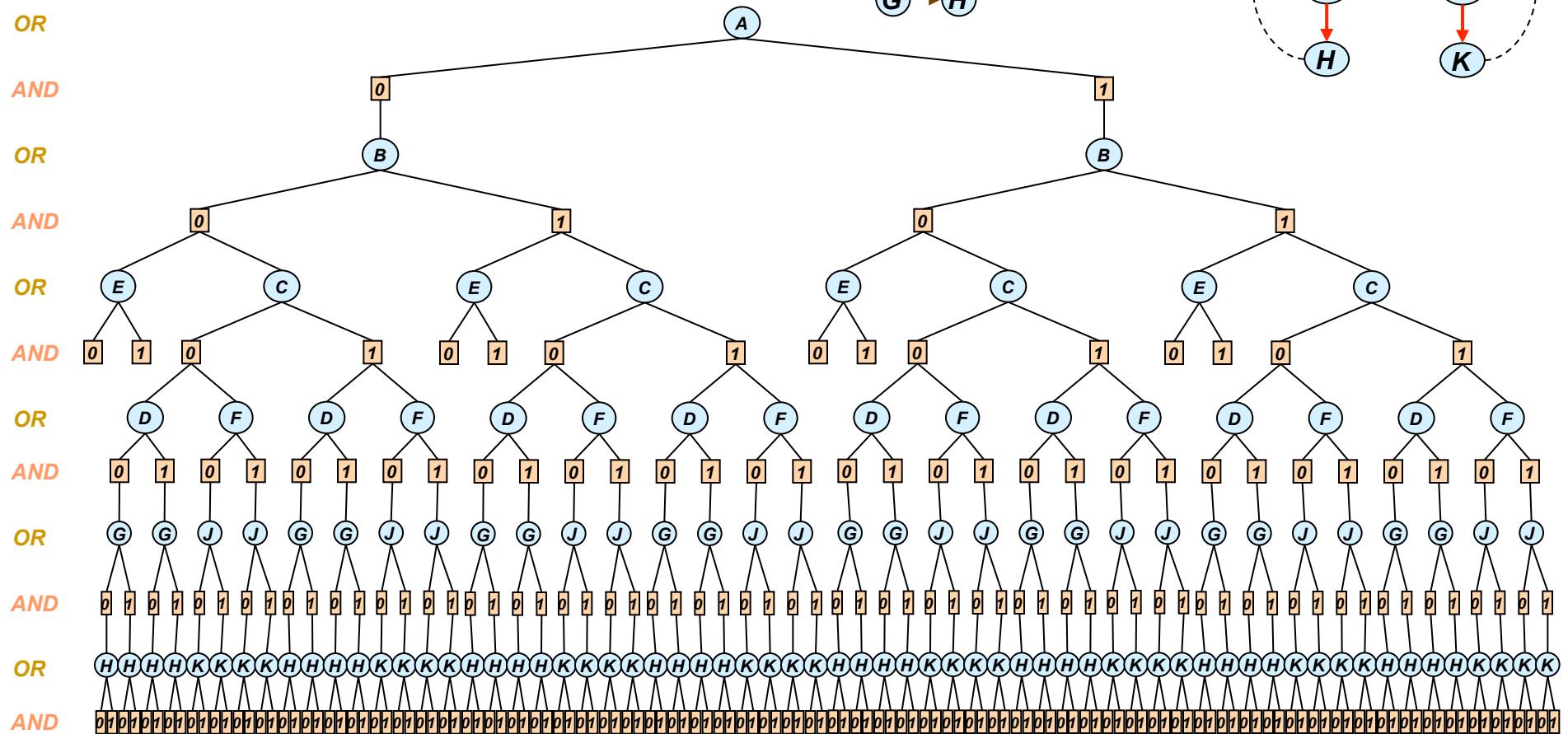


# From Search Trees to Search Graphs

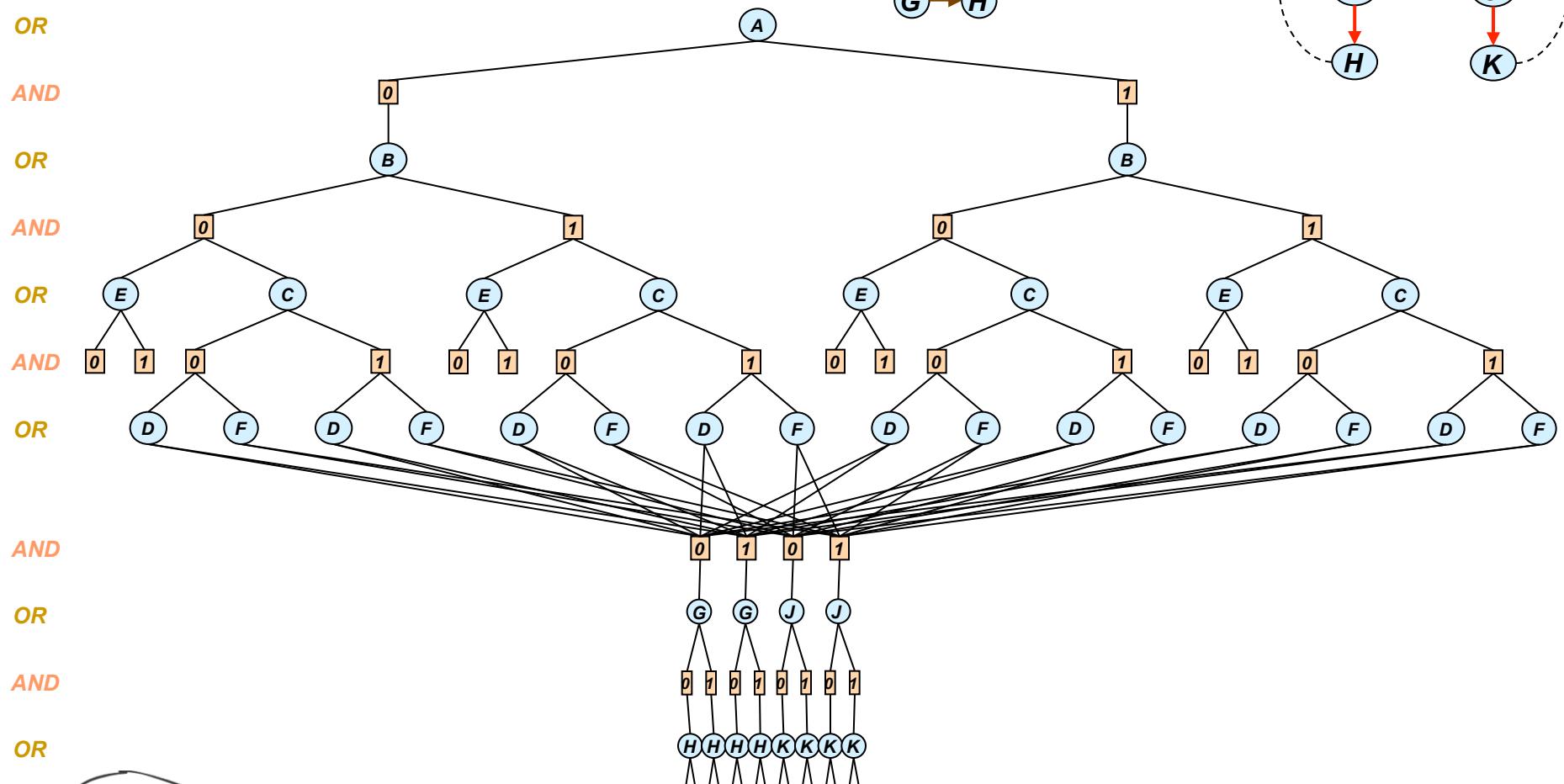
- Any two nodes that root **identical** sub-trees or sub-graphs can be **merged**



# From AND/OR Tree



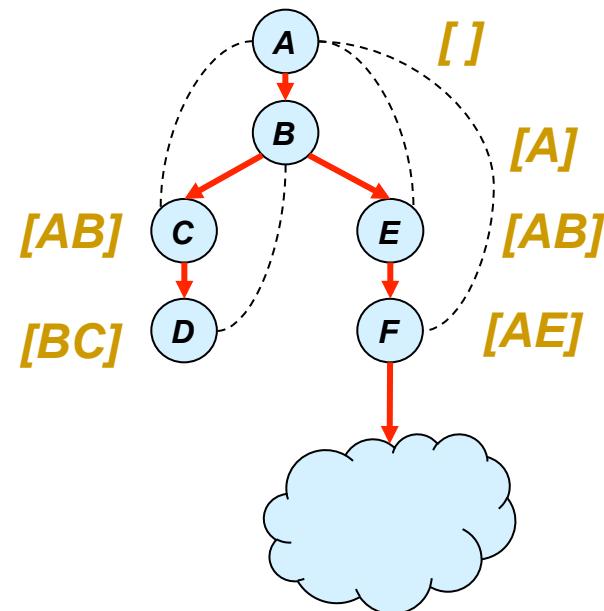
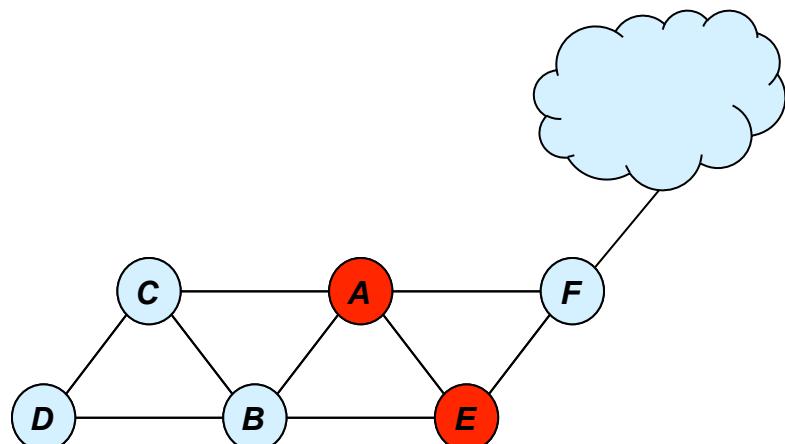
# An AND/OR Graph



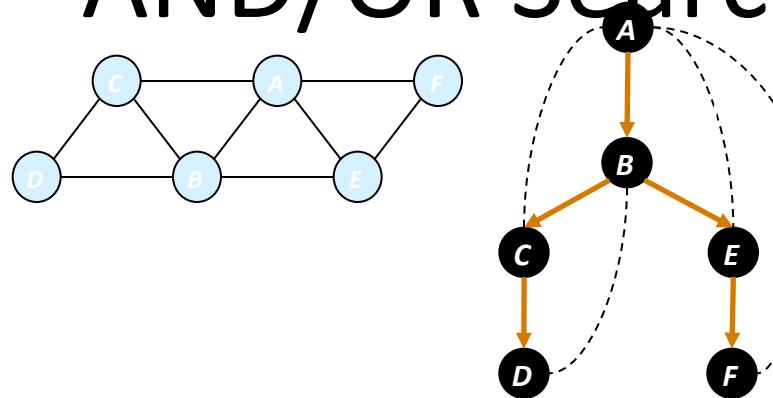
# Merging based on context

*context ( $X$ ) = ancestors of  $X$  connected to*

$\xrightarrow{X}$   
 $\xrightarrow{\text{descendants of } X}$

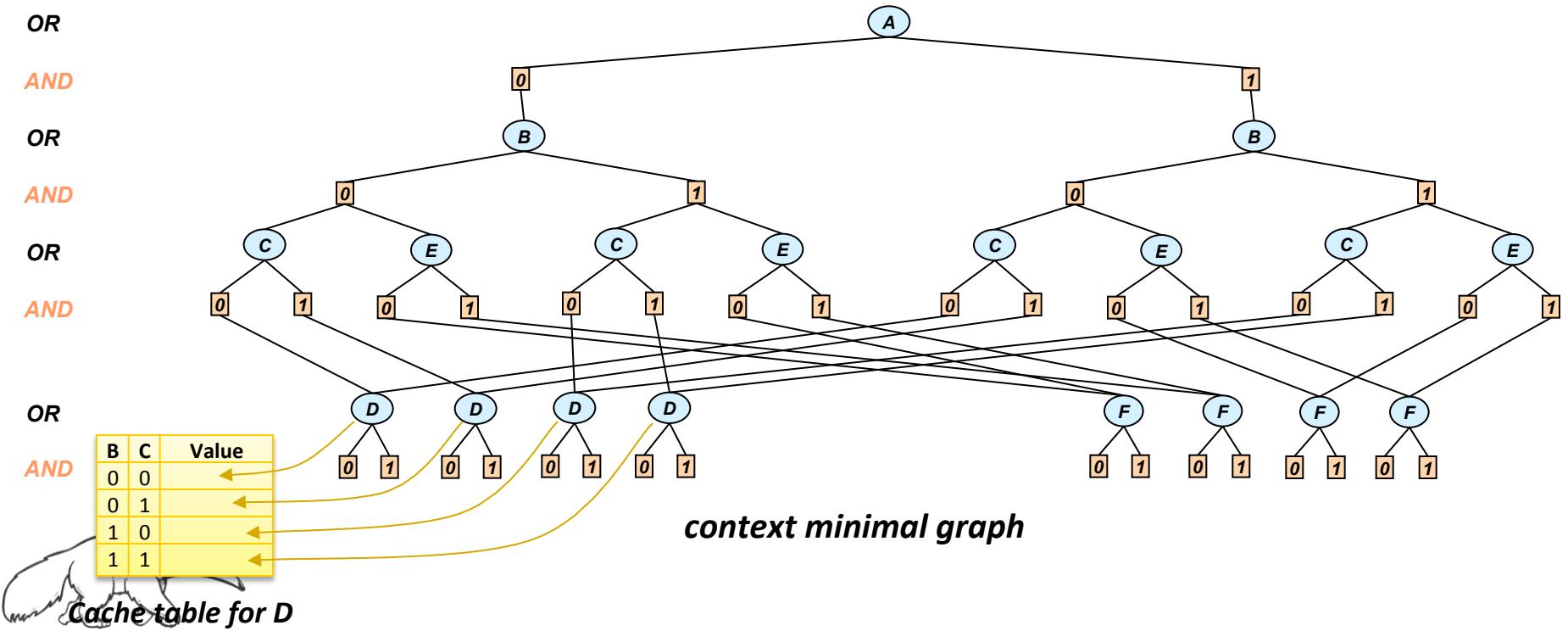


# AND/OR Search Graph



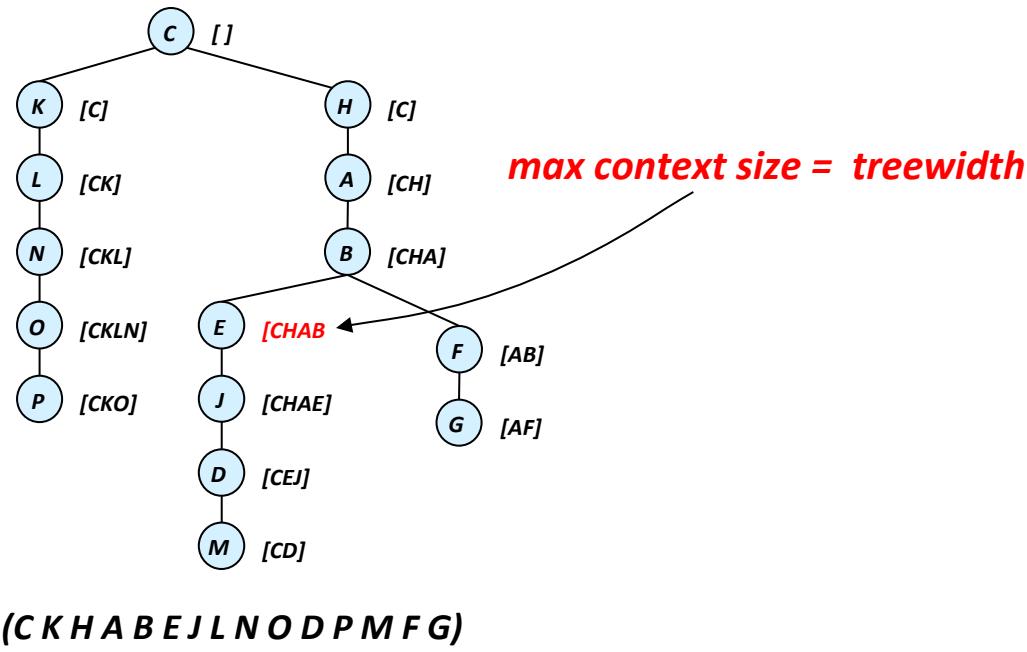
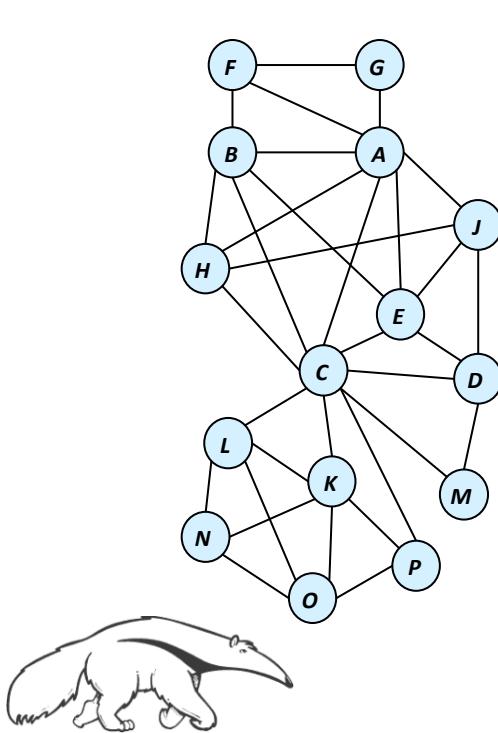
A	B	$f_1$	A	C	$f_2$	A	E	$f_3$	A	F	$f_4$	B	C	$f_5$	B	D	$f_6$	B	E	$f_7$	C	D	$f_8$	E	F	$f_9$				
0	0	2	0	0	3	0	0	0	0	0	2	0	0	0	0	0	4	0	0	3	0	0	1	0	0	1				
0	1	0	0	1	0	0	1	3	0	1	0	0	1	1	0	1	1	2	1	0	1	2	0	1	4	1	0	0		
1	0	1	1	0	0	1	0	2	1	0	0	1	0	1	2	1	1	4	1	1	0	1	0	1	0	1	1	0	1	
1	1	4	1	1	1	1	1	0	1	1	2	1	1	4	1	1	0	1	1	0	1	1	0	1	1	0	1	1	2	1

$$f(\mathbf{X}) = \min_X \sum_{i=1}^9 f_i(\mathbf{X})$$

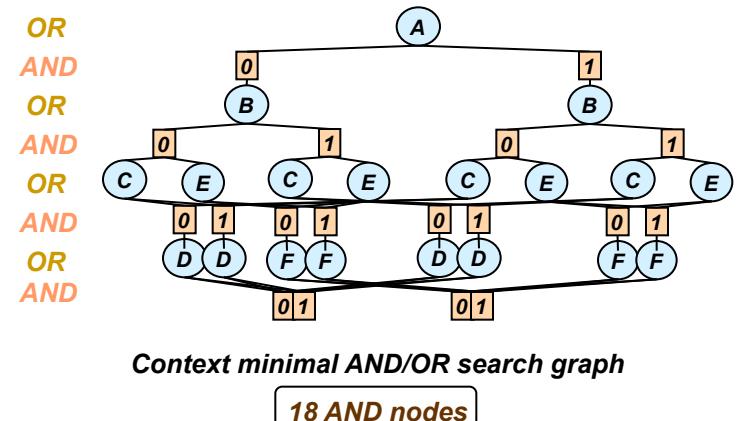
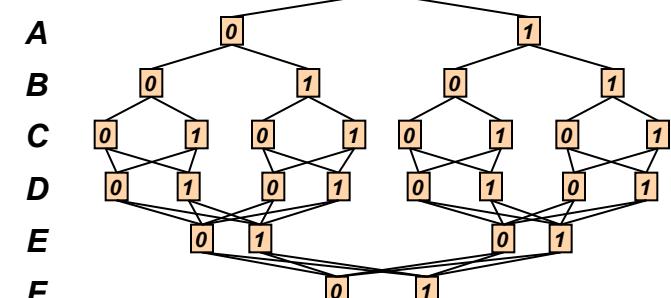
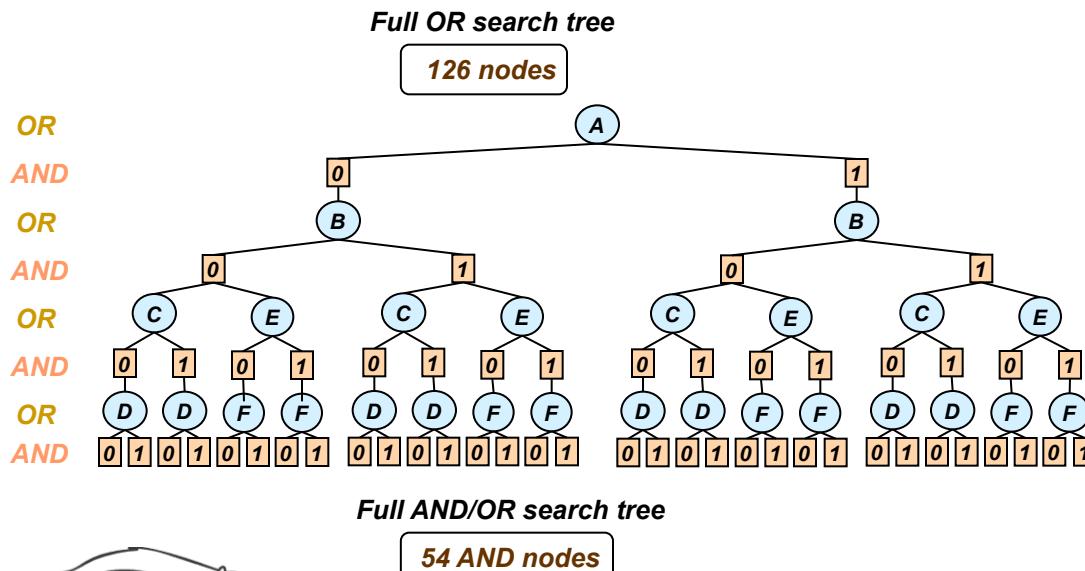
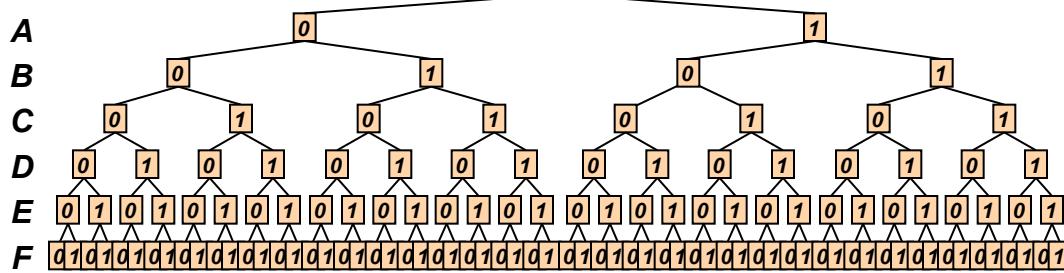
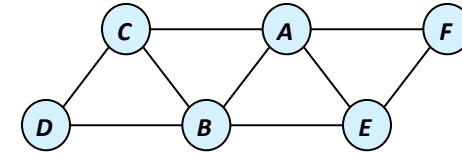


# How Big Is The Context?

**Theorem:** The maximum **context** size for a pseudo tree **is equal** to the **treewidth** of the graph along the pseudo tree.



# All Four Search Spaces



**Any query is best computed  
Over the c-minimal AO space**

# Complexity of AND/OR Graph Search

	AND/OR graph	OR graph
Space	$O(n k^{w^*})$	$O(n k^{pw^*})$
Time	$O(n k^{w^*})$	$O(n k^{pw^*})$

*k* = domain size

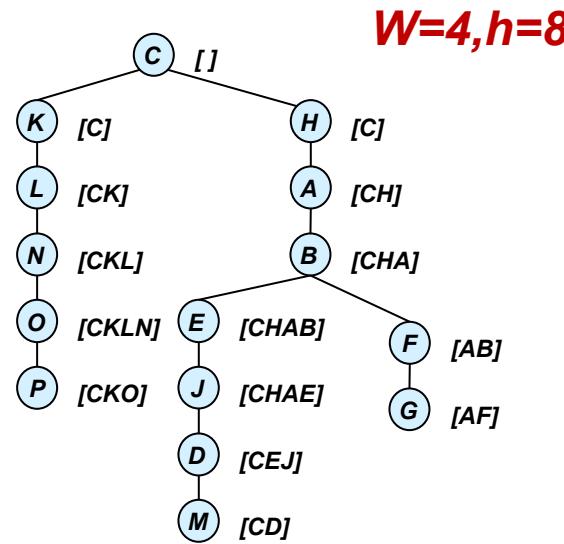
*n* = number of variables

*w\**= treewidth

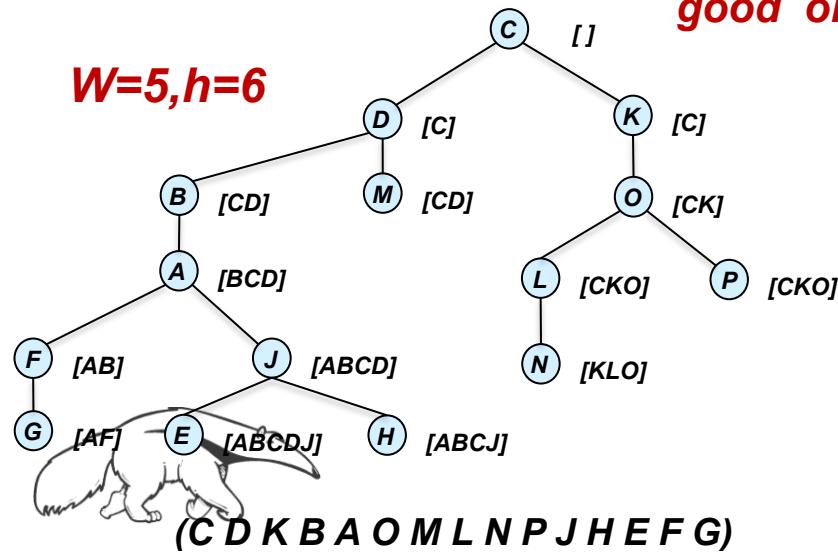
*pw\**= pathwidth



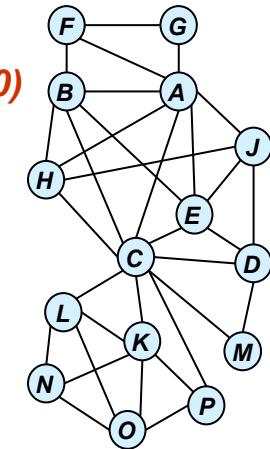
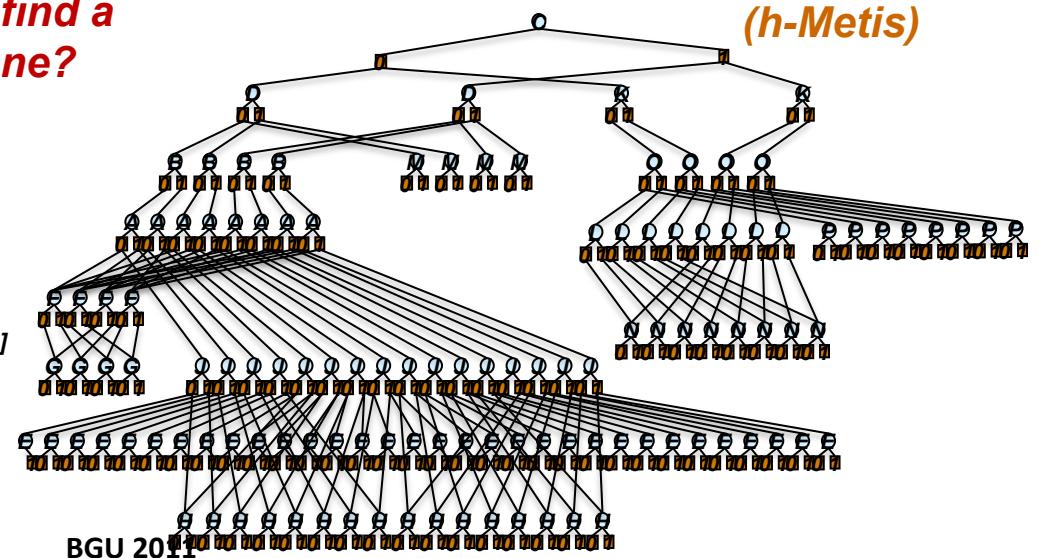
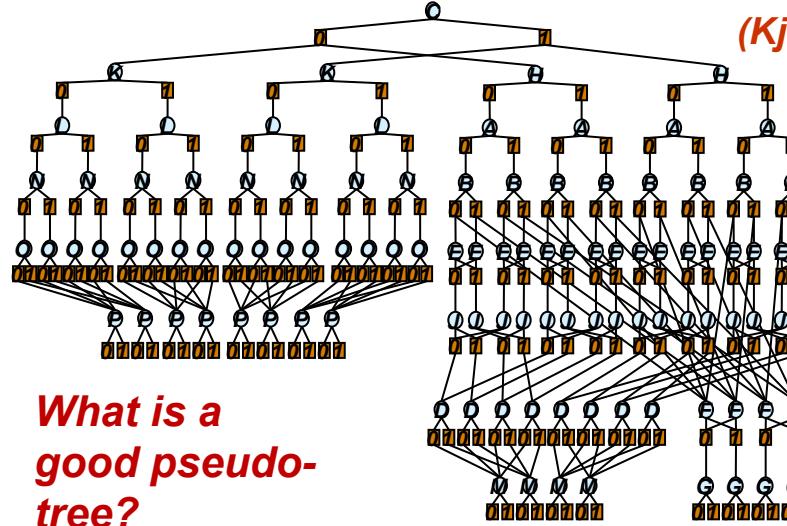
# The impact of the pseudo-tree



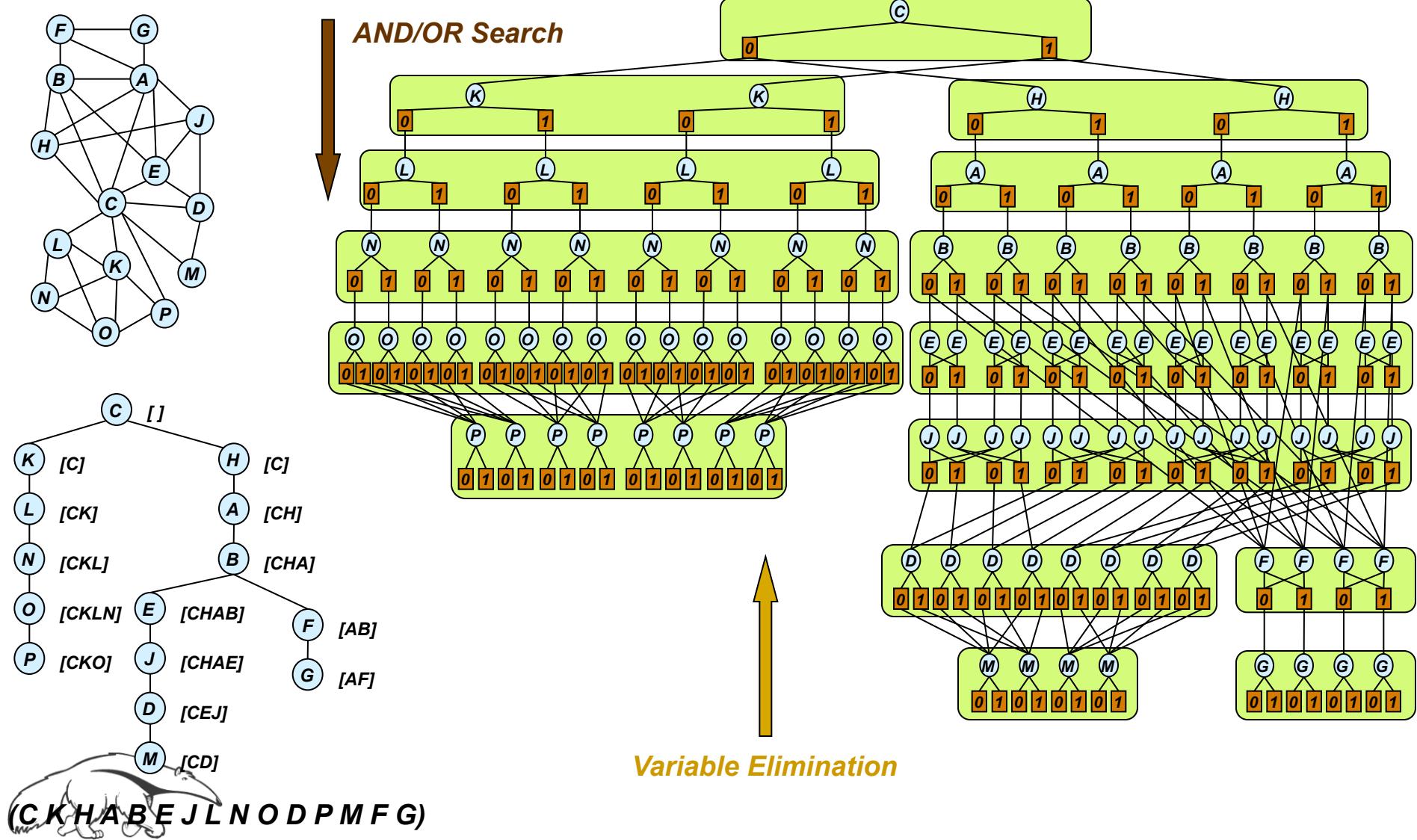
$W=5, h=6$



*What is a  
good pseudo-  
tree?  
How to find a  
good one?*



# AND/OR Context Minimal Graph



# Outline

- Graphical Models: reasoning principles
- OR Search Trees
- AND/OR Search Spaces for GM
- **AND/OR Branch-and-Bound and Best-First Search**
- Lower Bounding Heuristics
- Experimental evaluation
- Current work



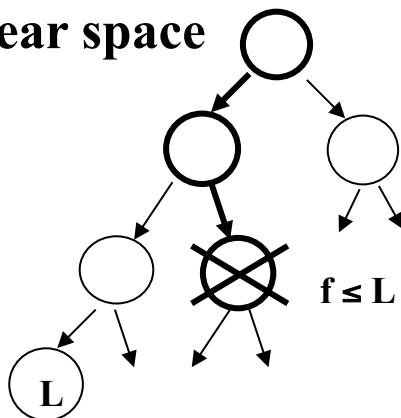
# Basic Heuristic Search Schemes

Heuristic function  $f(x)$  computes a lower bound on the best extension of  $x$  and can be used to guide a heuristic search algorithm. We focus on

## 1. Branch and Bound

Use heuristic function  $f(x^p)$  to prune the depth-first search tree.

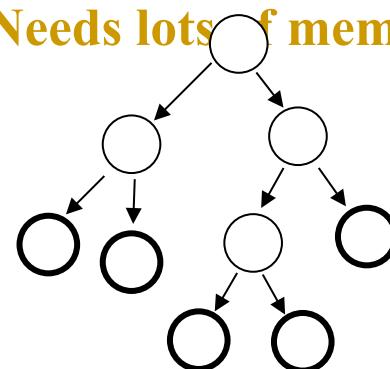
Linear space



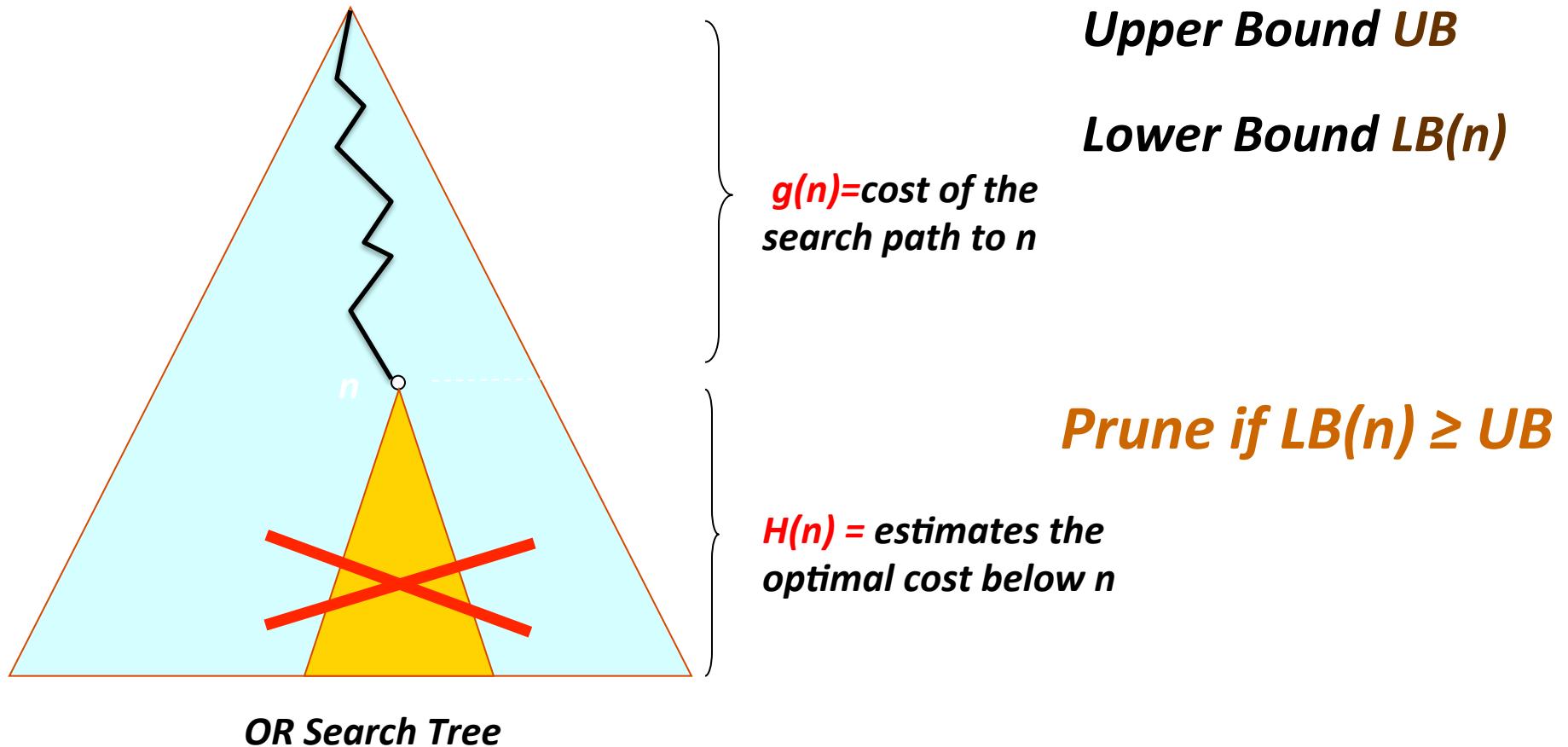
## 2. Best-First Search

Always expand the node with the highest heuristic value  $f(x^p)$ .

Needs lots of memory

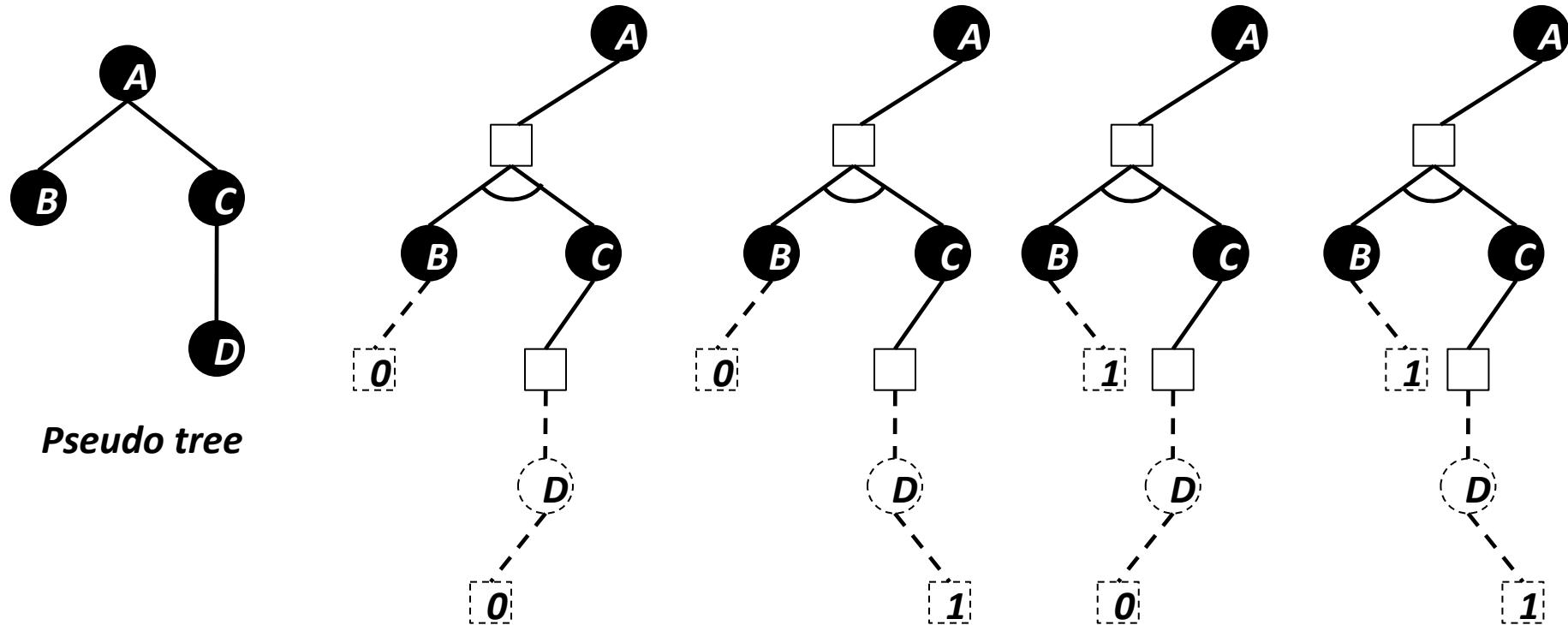


# Branch-and-Bound Search

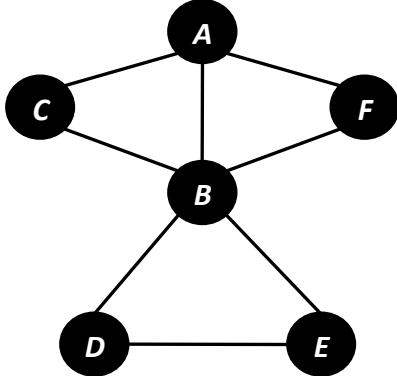


(Lawler & Wood66)

# Partial Solution Tree



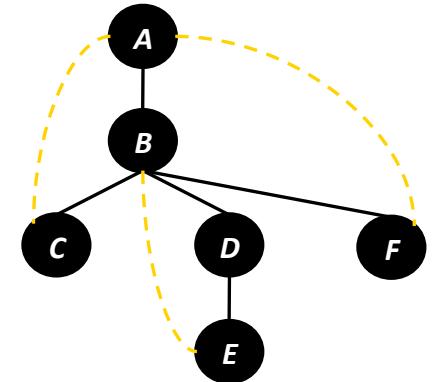
# Exact Evaluation Function



A	B	C	$f_1(ABC)$
0	0	0	2
0	0	1	5
0	1	0	3
0	1	1	5
1	0	0	9
1	0	1	3
1	1	0	7
1	1	1	2

A	B	F	$f_2(ABF)$
0	0	0	3
0	0	1	5
0	1	0	1
0	1	1	4
1	0	0	6
1	0	1	5
1	1	0	6
1	1	1	5

B	D	E	$f_3(BDE)$
0	0	0	6
0	0	1	4
0	1	0	8
0	1	1	5
1	0	0	9
1	0	1	3
1	1	0	7
1	1	1	4



OR

AND

OR

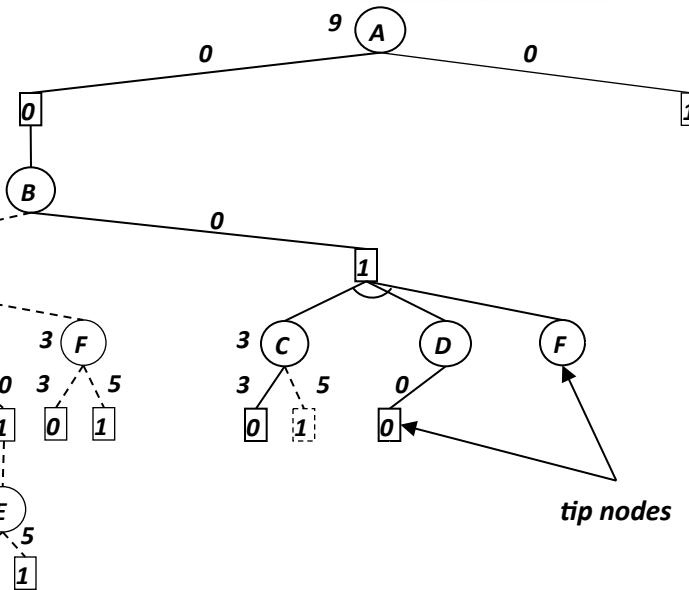
AND

OR

AND

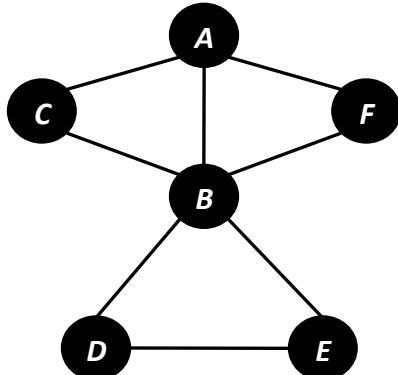
OR

AND



$$f^*(T') = w(A,0) + w(B,1) + w(C,0) + w(D,0) + v(D,0) + v(F)$$

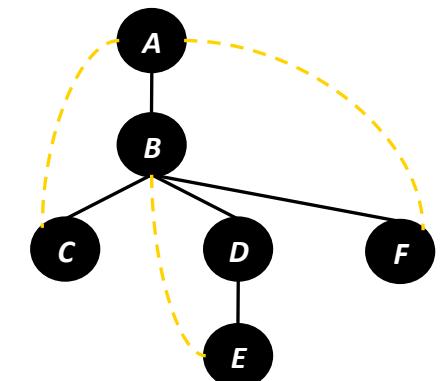
# Heuristic Evaluation Function



A	B	C	$f_1(ABC)$
0	0	0	2
0	0	1	5
0	1	0	3
0	1	1	5
1	0	0	9
1	0	1	3
1	1	0	7
1	1	1	2

A	B	F	$f_2(ABF)$
0	0	0	3
0	0	1	5
0	1	0	1
0	1	1	4
1	0	0	6
1	0	1	5
1	1	0	6
1	1	1	5

B	D	E	$f_3(BDE)$
0	0	0	6
0	0	1	4
0	1	0	8
0	1	1	5
1	0	0	9
1	0	1	3
1	1	0	7
1	1	1	4



OR

AND

OR

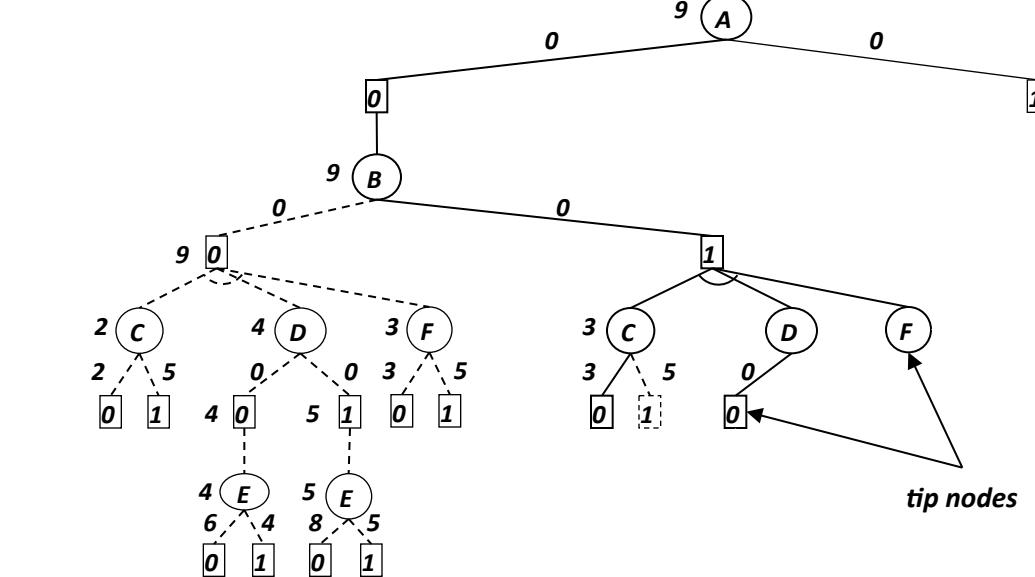
AND

OR

AND

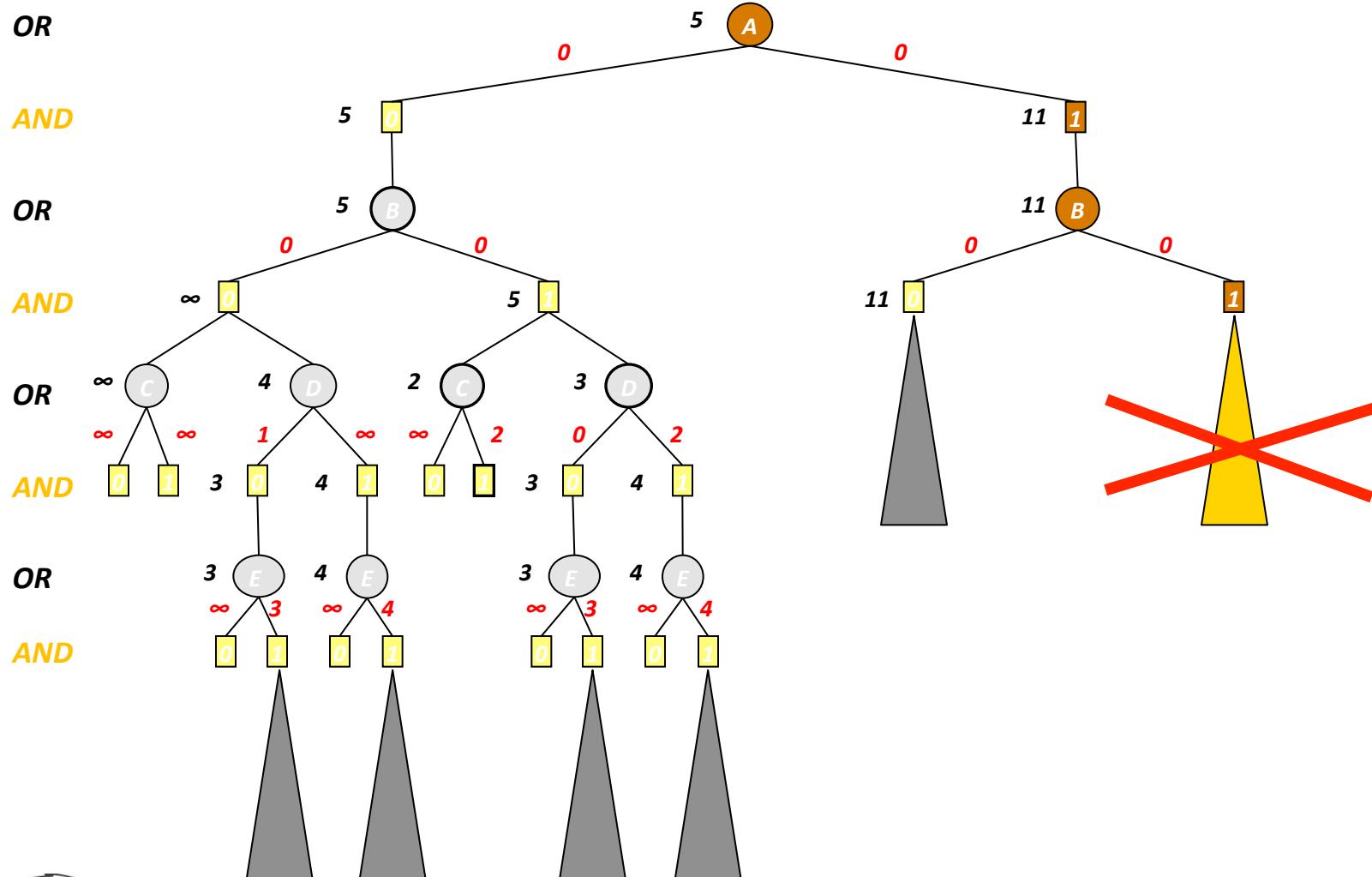
OR

AND



$$f(T') = w(A,0) + w(B,1) + w(C,0) + w(D,0) + h(D,0) + h(F) = 12 \leq f^*(T')$$

# AND/OR Branch-and-Bound Search



# Best-First Search Principle

- Best-first search expands first the node with the best heuristic evaluation function among all nodes encountered so far
- It **never** expands nodes whose evaluation function is beyond the optimal one, unlike depth-first search algorithms (Dechter & Pearl85)
- Superior among memory intensive algorithms employing the



# Best-First AND/OR Search

- Maintains the set of best partial solution trees
- **EXPAND** (top-down)
  - Traces down marked connectors from root (**best partial solution tree**)
  - Expands a tip node by generating its successors  $n'$
  - Associate each successor with heuristic estimate  $h(n')$ 
    - Initialize  $v(n') = h(n')$
- **REVISE** (bottom-up)
  - Updates node values  $v(n)$ 
    - OR nodes: **minimization**
    - AND nodes: **summation**
  - Marks the most promising solution tree from the root
  - Label the nodes as SOLVED:
    - OR is SOLVED if marked child is SOLVED
    - AND is SOLVED if all children are SOLVED
- Terminate **when root** node is **SOLVED**



[specializes Nilsson's AO\* to graphical models (Nilsson80)]

# Outline

- Graphical Models: reasoning principles
- OR Search Trees
- AND/OR Search Spaces for GM
- AND/OR Branch-and-Bound and Best-First Search
- Lower Bounding Heuristics
- Experimental evaluation
- Current work



# How to Generate Heuristics *(Pearl86)*

- The principle of relaxed models
  - Linear relaxation for integer programs
  - Mini-Bucket Elimination for graphical models
  - Bounded directional consistency ideas
  - Pattern databases



# Inference for Optimization: Bucket Elimination

*Algorithm BE-mpe (Dechter 1996, Bertele and Brioche, 1977)*

$$MPE = \max_{a,e,d,c,b} P(a)P(c|a)P(b|a)P(d|a,b)P(e|b,c)$$

*bucket B:*

$$\max_X \prod \underbrace{P(b|a) \quad P(d|b,a) \quad P(e|b,c)}_{h^B(a, d, c, e)}$$

*bucket C:*

$$P(c|a) \quad h^B(a, d, c, e) \quad h^c(a, d, e)$$

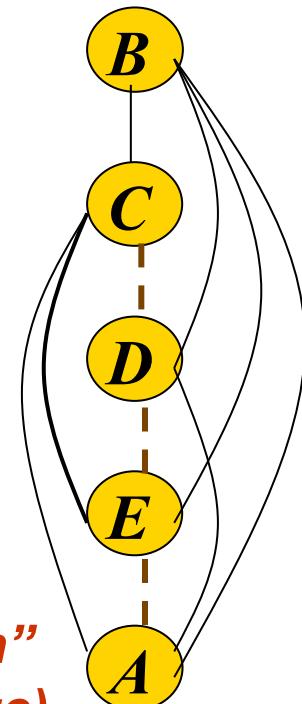
*bucket D:*

$$e=0 \quad h^c(a, d, e) \quad h^D(a, e)$$

*bucket E:*

$$P(a) \quad h^D(a, e) \quad h^E(a) \quad P(a|e=0)$$

$W^*=4$   
*"induced width"*  
*(max clique size)*



# Mini-bucket approximation: MPE task

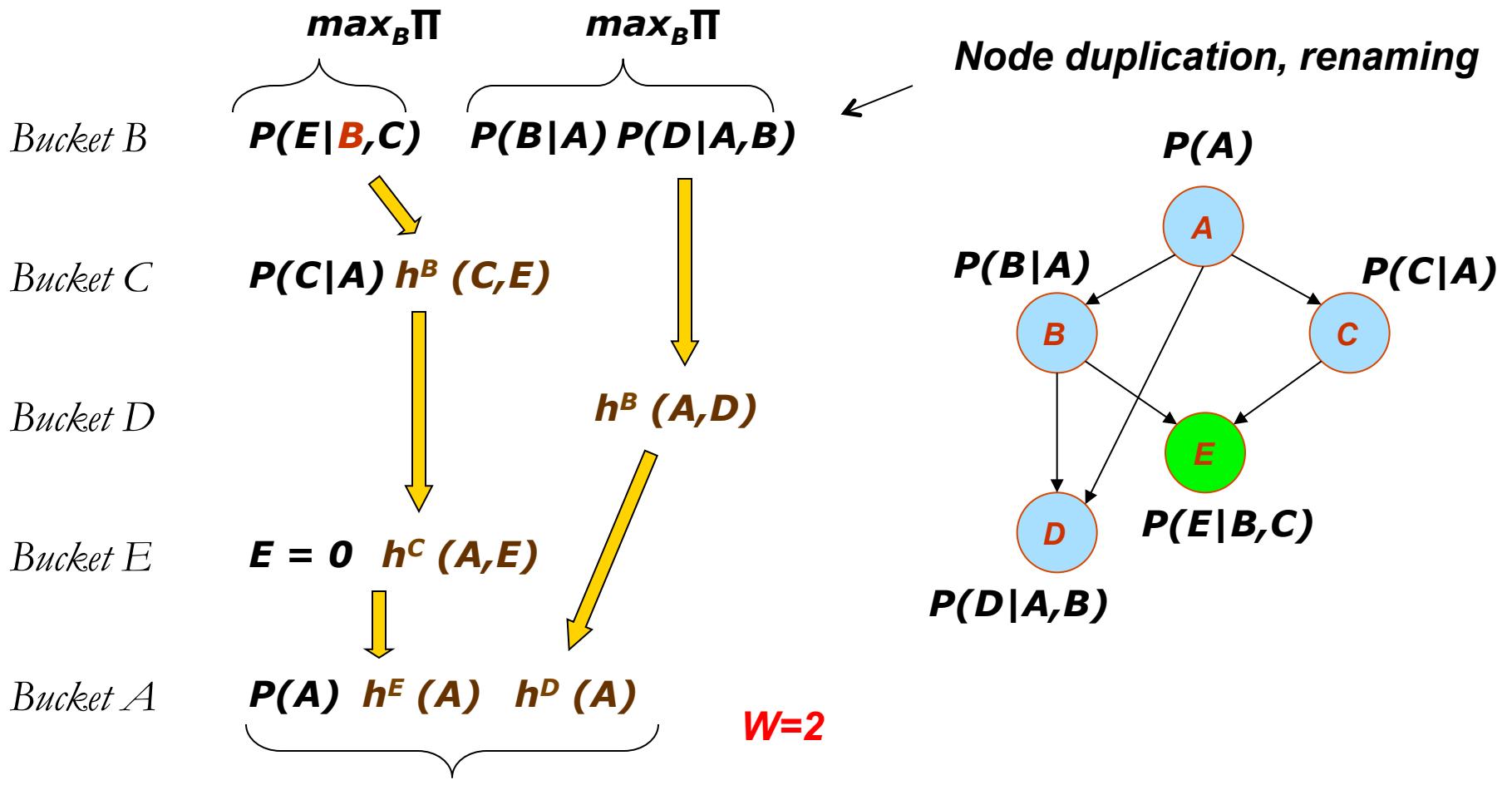
*Split a bucket into mini-buckets => bound complexity*

$$\begin{aligned}
 \textbf{bucket}(\mathbf{X}) &= \\
 \underbrace{\{ h_1, \dots, h_r, h_{r+1}, \dots, h_n \}}_{h^X = \max_X \prod_{i=1}^n h_i} &\quad \downarrow \\
 \underbrace{\{ h_1, \dots, h_r \}} &\quad \underbrace{\{ h_{r+1}, \dots, h_n \}} \\
 g^X = (\max_X \prod_{i=1}^r h_i) \cdot (\max_X \prod_{i=r+1}^n h_i) &\quad \downarrow \\
 \boxed{h^X \leq g^X}
 \end{aligned}$$

Exponential complexity decrease :  $O(e^n) \rightarrow O(e^r) + O(e^{n-r})$

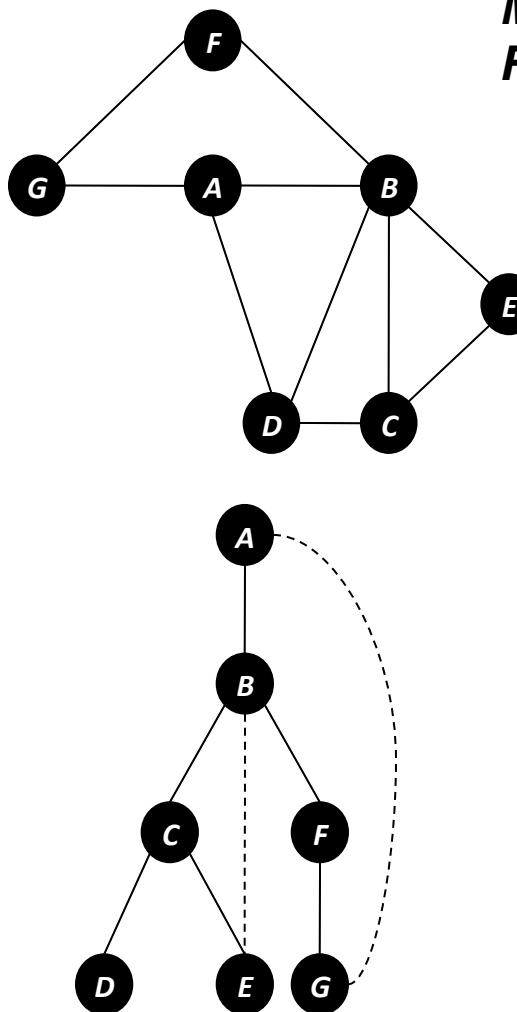


# Mini-Bucket Elimination

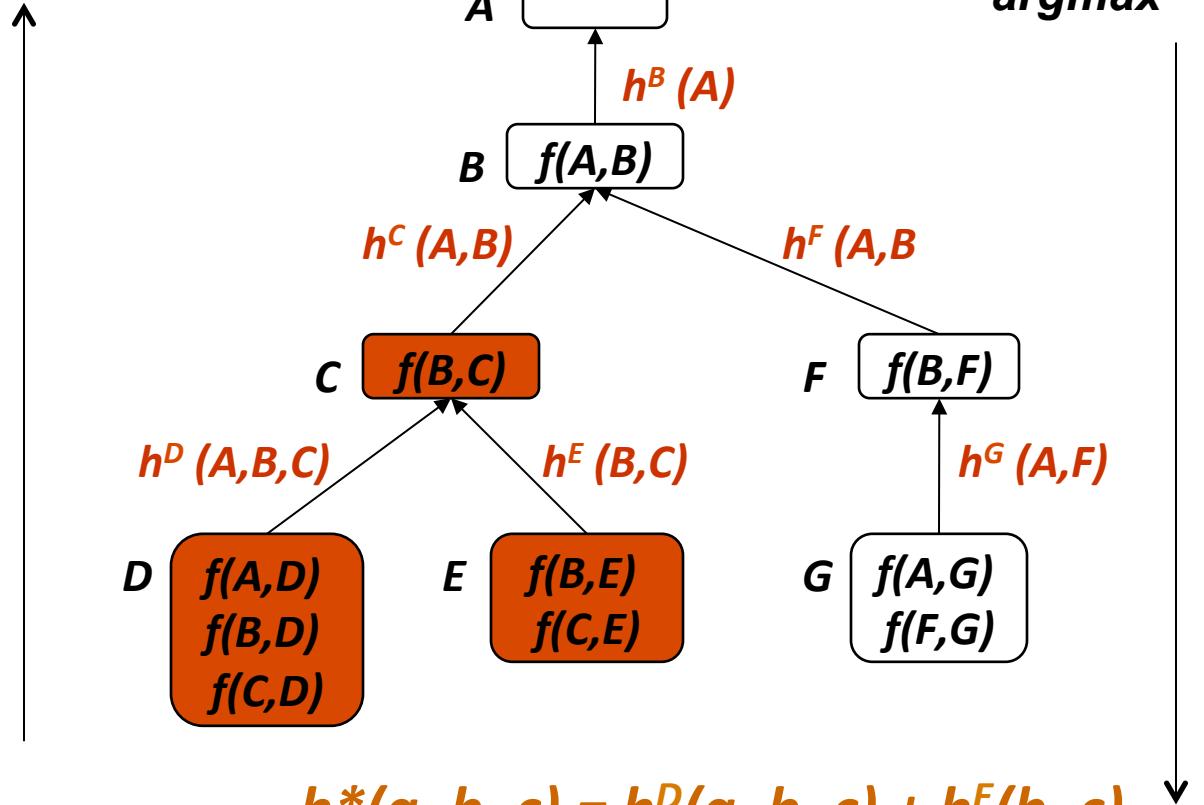


# Bucket Elimination

$$\min_{a,b,c,d,e,f,g} f(a,b) + f(a,d) + f(b,c) + f(a,d) + f(b,d) + f(c,d) + f(b,e) + f(c,e) + f(b,f) + f(a,g) + f(f,g) =$$



*Messages  
Finding max*

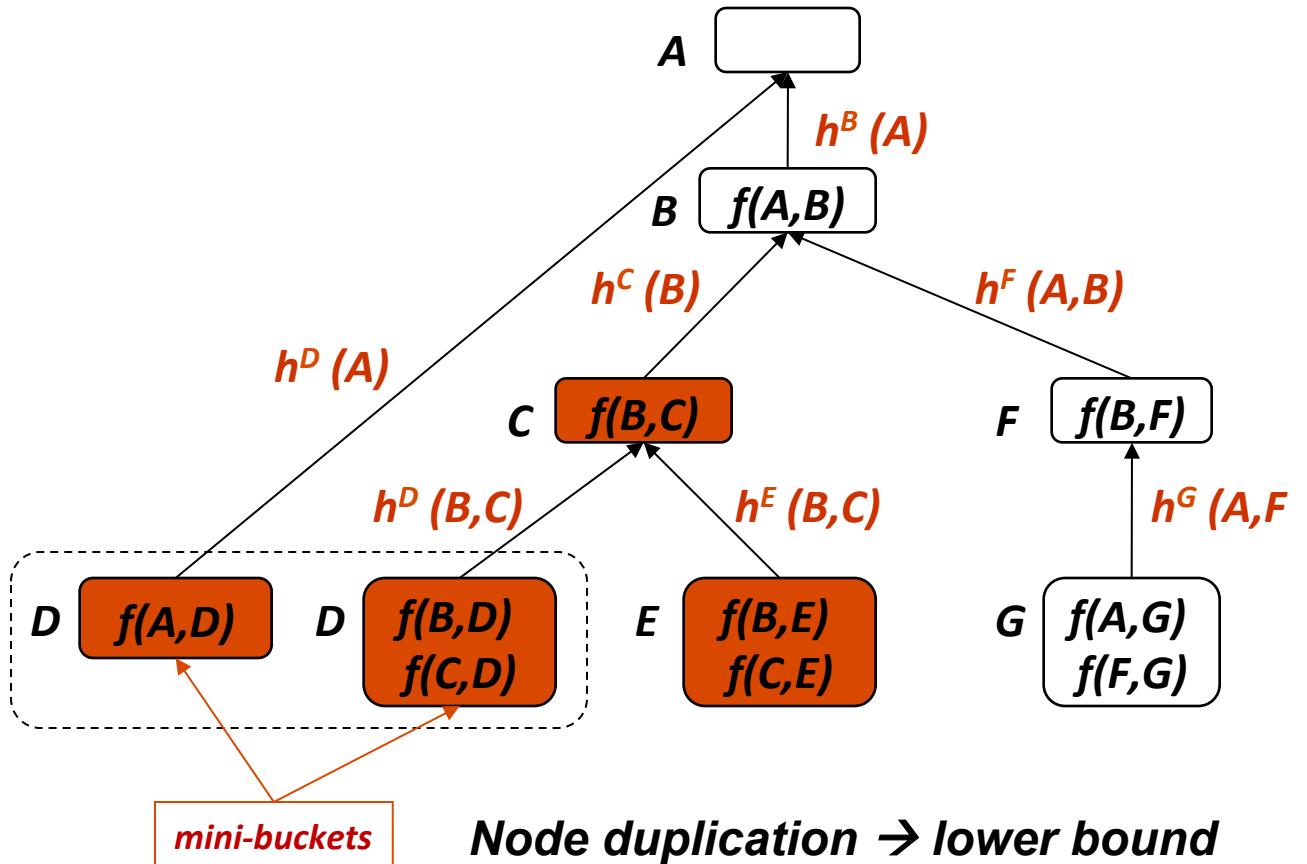
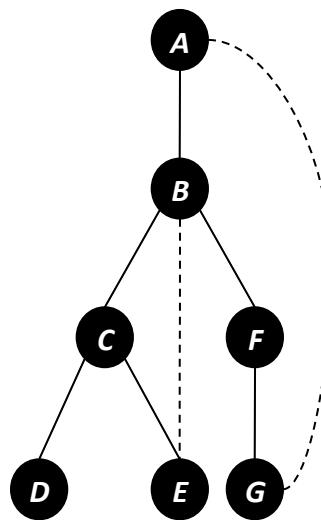
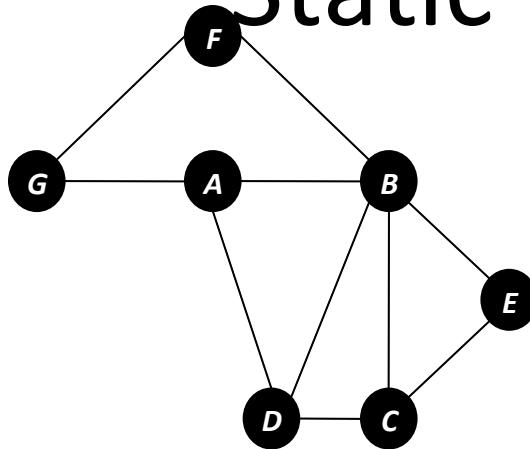


$$h^*(a, b, c) = h^D(a, b, c) + h^E(b, c)$$

*Ordering: (A, B, C, D, E, F, G)*



# Static Mini-Bucket Heuristics



$$\begin{aligned}
 h(a, b, c) &= h^D(a) + h^D(b, c) + h^E(b, c) \\
 &\leq h^*(a, b, c)
 \end{aligned}$$

Ordering: (A, B, C, D, E, F, G)

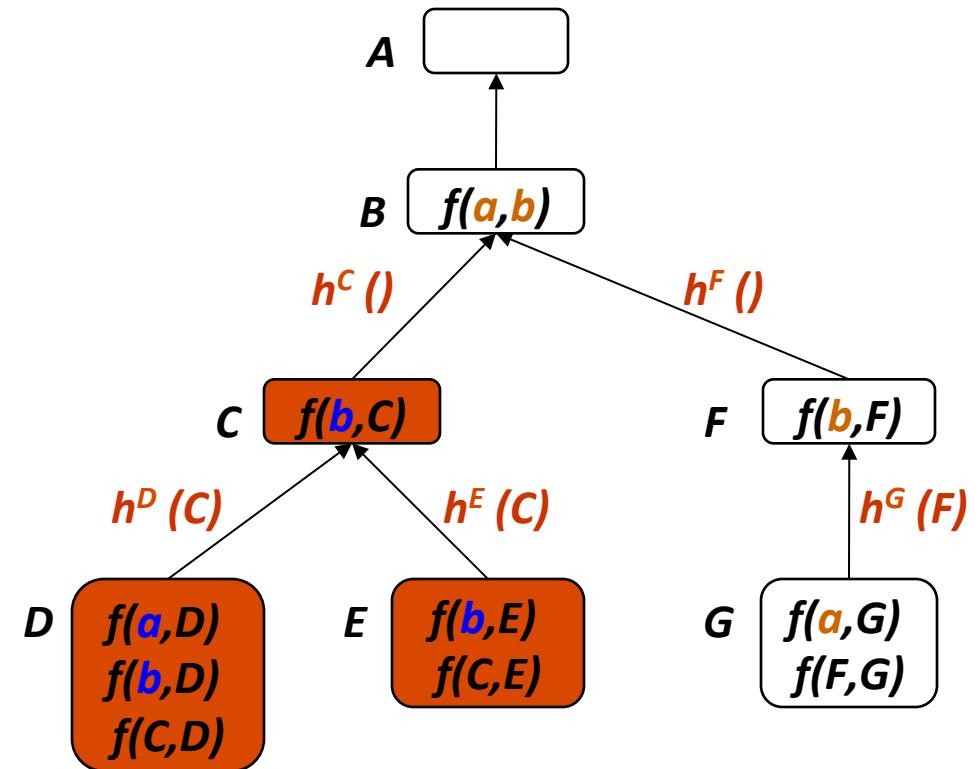
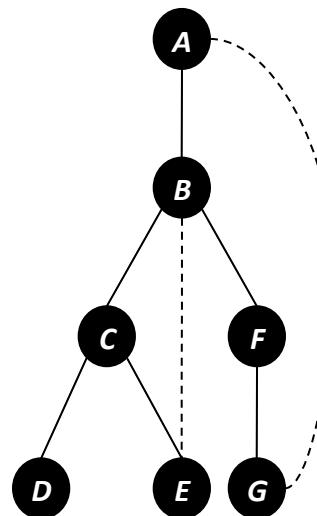
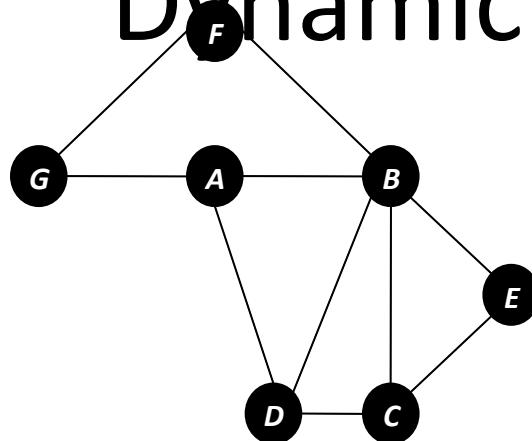


# Mini-Bucket Elimination

- Approximation of the Bucket Elimination algorithm by partitioning large buckets into “mini-buckets” which are processed separately (Dechter & Rish97)
- Properties
  - Parameterized by i-bound (controls complexity)
  - Computes a lower bound on the exact solution
  - Approximation improves with the i-bound



# Dynamic Mini-Bucket Heuristics



$$\begin{aligned}
 h(a, b, c) &= h^D(c) + h^E(c) \\
 &= h^*(a, b, c)
 \end{aligned}$$

Ordering: (A, B, C, D, E, F, G)



# Outline

- Graphical Models: reasoning principles
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# What are the empirical questions?

- What is the
  - Impact of AND/OR decomposition?
  - Impact of caching (Tree search vs graph search)?
  - The heuristic strength vs. search tradeoff.
  - impact of depth-first BB vs Best-first
  - The (w,h) of the pseudo-tree



# Experiments

- Optimization task
  - Most Probable Explanation in belief networks
  - Optimal wcsp
- Algorithms
  - AOBB-C+SMB(i): AOBB w/ full caching and mini-buckets
  - AOBF-C+SMB(i): AOBF w/ full caching and mini-buckets
  - Samlam (Recursive Conditioning) (Darwiche01)
  - Superlink (genetic linkage analysis) (Fishelson&Geiger02)
  - ILOG CPLEX 11.0
- Benchmarks
  - ISCAS'89 circuits
  - Grid networks
  - Genetic linkage analysis
  - Mastermind games



# Grid Networks (BN)

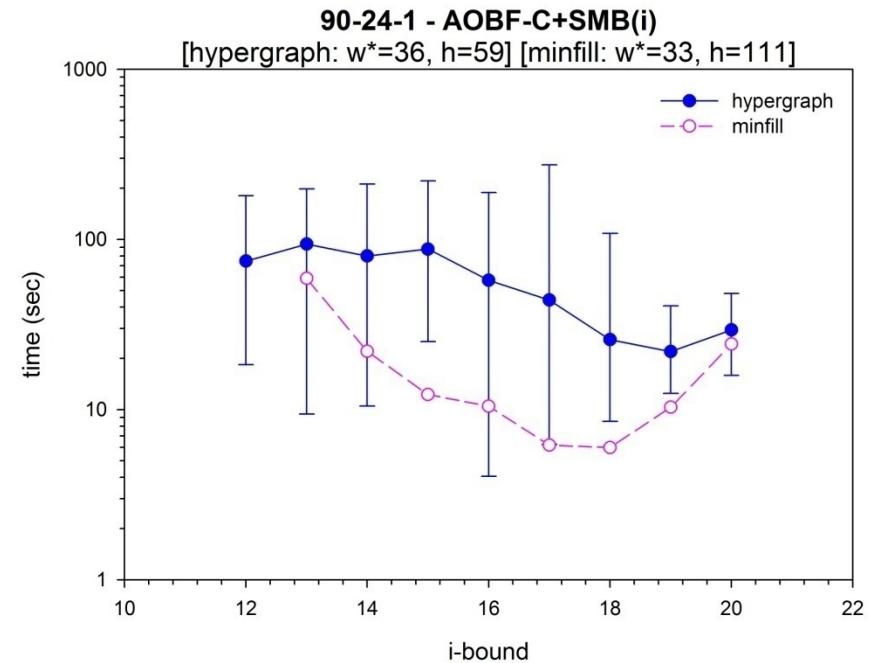
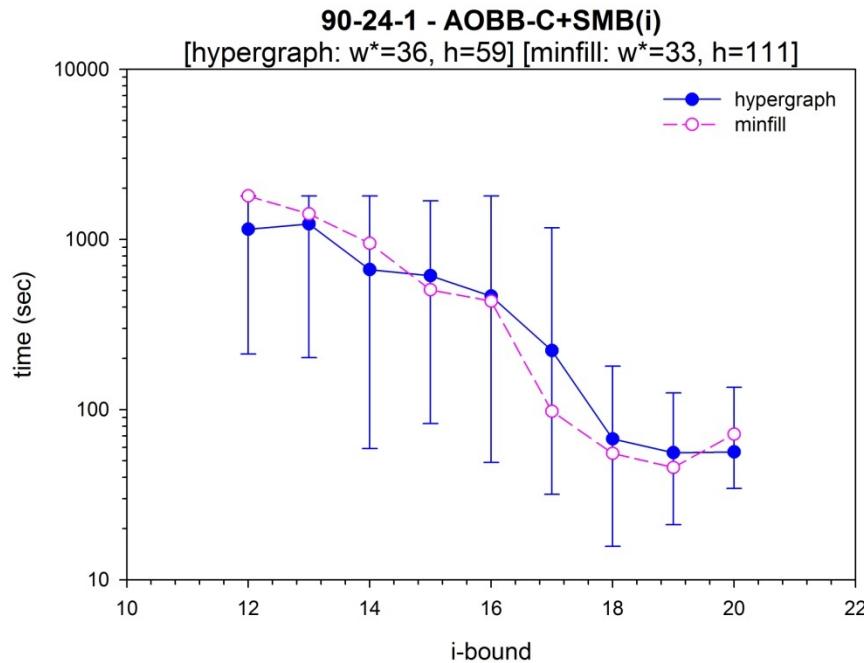
(Sang et al.05)

grid (w*, h) (n, e)	Samlam	MBE(i) BB-C+SMB(i)		MBE(i) BB-C+SMB(i)		MBE(i) BB-C+SMB(i)		MBE(i) BB-C+SMB(i)	
		AOBB+SMB(i) AOBB-C+SMB(i) AOBF-C+SMB(i)		AOBB+SMB(i) AOBB-C+SMB(i) AOBF-C+SMB(i)		AOBB+SMB(i) AOBB-C+SMB(i) AOBF-C+SMB(i)		AOBB+SMB(i) AOBB-C+SMB(i) AOBF-C+SMB(i)	
		i=12	i=12	i=14	i=14	i=16	i=16	i=18	i=18
		time	nodes	time	nodes	time	nodes	time	nodes
90-24-1 (33, 111) (576, 20)	out	0.28		0.64		1.69		4.60	
		-	-	-	-	-	-	-	-
		-	-	2338.67	24,117,151	1548.09	18,238,983	138.67	1,413,764
90-34-1 (45, 153) (1154, 80)	out	-	-	1273.09	9,047,518	596.27	4,923,760	70.42	473,675
		-	-	21.94	75,637	10.59	33,770	6.06	5,144
		0.63		1.25		3.72		11.66	
90-38-1 (47, 163) (1444, 120)	out	-	-	-	-	-	-	-	-
		-	-	-	-	-	-	-	-
		-	-	-	-	-	-	-	-
	out	out		243.63	596,978	270.88	667,013		
		0.78		1.67		4.20		12.36	
		-	-	-	-	-	-	-	-
	out	2032.33	6,835,745	-	-	807.38	2,850,393	568.69	2,079,146
		969.02	2,623,971	1753.10	3,794,053	203.67	614,868	165.45	488,873
		101.69	174,786	103.80	146,237	54.00	95,511	53.44	78,431



*Min-fill pseudo tree. Time limit 1 hour.*

# Impact of the Pseudo Trees and heuristic power



*Runtime distribution for AOBB and AOBF with different i-bound for  
The mini-bucket heuristics for pseudo-trees created by hypergraph and min-fill  
over 20 independent runs for 90-24-1 grid instance.*



# Genetic Linkage Analysis

(Fishelson & Geiger02)

pedigree (w*, h) (n, d)	Samlam Superlink	MBE(i)		MBE(i)		MBE(i)		MBE(i)	
		BB-C+SMB(i)	AOBB+SMB(i)	BB-C+SMB(i)	AOBB+SMB(i)	BB-C+SMB(i)	AOBB+SMB(i)	BB-C+SMB(i)	AOBB+SMB(i)
		i=12	time	i=14	time	i=16	time	i=18	time
ped30 (23, 118) (1016, 5)	out	-	0.42	-	0.83	-	1.78	-	5.75
	13095.83	10212.70	93,233,570	8858.22	82,552,957	-	-	-	-
	out		out		out	out		30.39	72,798
ped33 (37, 165) (581, 5)	out	0.58	-	2.31	-	7.84	-	33.44	-
	2804.61	34,229,495	737.96	9,114,411	3896.98	50,072,988	159.50	1,647,488	-
	-	1426.99	11,349,475	307.39	2,504,020	1823.43	14,925,943	86.17	453,987
	out			140.61	407,387	out		74.86	134,068
ped42 (25, 76) (448, 5)	out	4.20	-	31.33	-	96.28	-	out	-
	561.31	-	-	-	-	2364.67	22,595,247		
	out		out			133.19	93,831		



*Min-fill pseudo tree. Time limit 3 hours.*

# ISCAS'89 Benchmark (WCSP)

iscas (w*, h) (n, d)	MBE(i)		MBE(i)		MBE(i)		MBE(i)		toolbar	
	BB-C+SMB(i)	AOBB+SMB(i)	BB-C+SMB(i)	AOBB+SMB(i)	BB-C+SMB(i)	AOBB+SMB(i)	BB-C+SMB(i)	AOBB+SMB(i)	toolbar-BTD	nodes
	i=8	i=10	i=10	i=12	i=12	i=14	i=14			time
	time	nodes	time	nodes	time	nodes	time	nodes	time	nodes
<b>c499</b> (23, 55) (499, 2)	0.08	-	0.08	-	0.14	-	0.28	-	-	-
	-	-	-	-	1.53	4,495	6.20	35,314	-	-
	96.46	1,265,425	39.65	526,517	1.42	18,851	37.26	486,656	100.96	1,203,734
	19.28	99,906	7.36	40,285	0.47	2,401	5.83	34,708		
	3.91	14,049	2.45	8,816	0.34	1,032	2.52	8,755		
<b>s1196</b> (54, 97) (562, 2)	0.16	-	0.19	-	0.38	-	0.94	-	-	-
	-	-	-	-	-	-	-	-	-	-
	-	-	1347.95	12,392,442	-	-	1949.37	15,775,180	376.35	1,276,514
	3347.38	13,554,137	503.30	2,425,152	2299.72	11,488,366	734.66	3,524,780		
	22.67	72,075	2.89	9,336	13.02	40,210	7.27	21,989		
<b>s1238</b> (59, 94) (541, 2)	0.16	-	0.22	-	0.38	-	0.92	-	-	-
	-	-	-	-	-	-	-	-	-	-
	-	-	-	-	1722.53	18,302,873	1394.86	14,213,319	-	-
	1897.37	8,386,634	1682.99	7,431,223	281.05	1,350,933	248.27	1,220,658		
	34.09	137,960	29.41	111,205	12.31	53,095	6.64	26,101		



# UAI 2010 evaluation, 2008, 2006

- Toulbar2: INRA

**Summary:** Toulbar2 is an open source exact anytime Weighted CSP solver using Branch and Bound and soft local consistency

**Team members:** S. de Givry, D. Allouche, A. Favier, T. Schiex

**Additional contributors:** M. Sanchez, S. Bouveret, H. Fargier, F. Heras, P. Jegou, J. Larrosa, K. L. Leung, S. N'diaye, E. Rollon, C. Terrioux, G. Verfaillie, M. Zytnicki

**Contact person:** Thomas Schiex, Thomas.Schiex@toulouse.inra.fr

Detailed description

- Daoopt: UCI Irvine

**Summary:** "daoopt" and "daoopt.anytime" are based on AND/OR branch and bound graph search, with mini bucket heuristics and LDS (Limited Discrepancy Search) initialization.

**Team members:** Lars Otten, Rina Dechter

**Additional Contributor:** Radu Marinescu

**Contact person:** Lars Otten, lotten@ics.uci.edu

Detailed description

**Web-site:** <http://graphmod.ics.uci.edu>

***3<sup>rd</sup> in all 3 categories  
After Toolbar, Joris***



# What did we learn

- Use the highest heuristic memory allows
- Generate heuristic in pre-processing
- Use AOBB with caching (best-first run out of memory). We also have adaptive-caching
- Try to get the best induced-width pseudo-tree
- Use some good initial upper-bound from local search



# Outline

- Graphical Models: reasoning principles
- OR Search Trees
- AND/OR Search Spaces for GM
- AND/OR Branch-and-Bound and Best-First Search
- Lower Bounding Heuristics
- Experimental evaluation
- Current work



# Recent related highlights

- Improving Heuristics due to “moment matching” or soft arc-consistency. (Flerova, Ihler, Dechter, Otten, 2011)
- Anytime behavior of AOBB (Otten and Dechter, SOCS 2011)
- Improving treewidth (Kask et. Al. 2011)
- Improving mini-bucket partitioning (Rollon 2010)



## *Bounding algorithms*

***non-iterative  
message-passing  
schemes***

e.g. **MBE** [Dechter, Rish 2003]

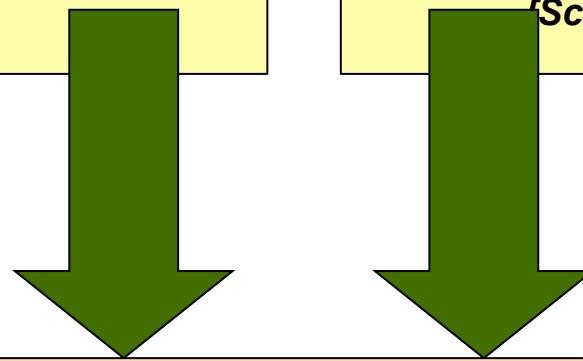
***iterative schemes  
using re-parametrization***

e.g. **MPLP** [Globerson et al. 2007],

**Max-sum diffusion** [Kovalevsky et al. 1975]

**Soft arc-consistency**

[Schiex 2000, Bistarelli et al. 2000]



***Mini-Bucket with moment-matching***



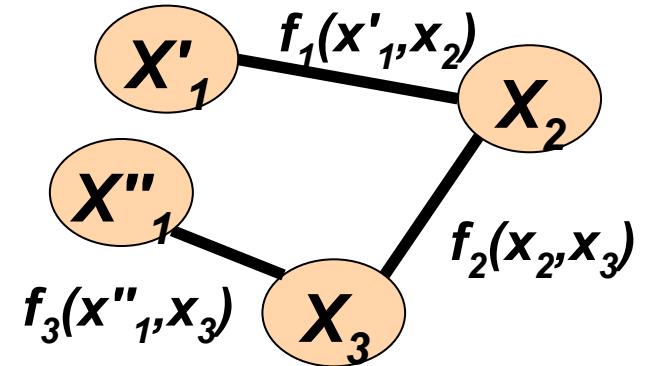
# Intuition behind MBE-MM

***How to make max-marginals equal?***

***Do cost shifting!***

$$C_1(x_2, x_3) = \max_{x_1} f_1(x_1, x_2) \cdot f_3(x_1, x_3)$$

$$C_1(x_2, x_3) = \max_{x_1} f_1(x_1, x_2) g(x_1) \cdot f_3(x_1, x_3) / g(x_1)$$

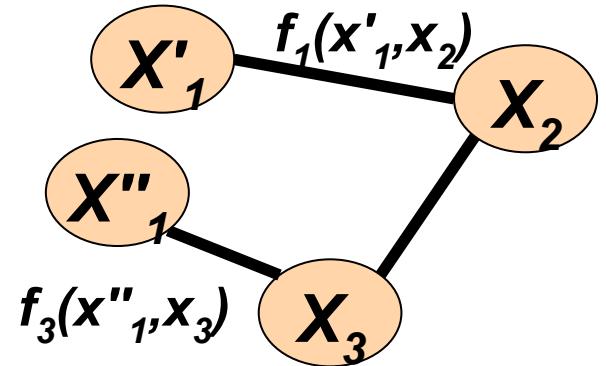


# Intuition behind MBE-MM

$$x_1^{*''} = \operatorname{argmax}_{x'_1} \max_{x_2} [f_1(x'_1, x_2) \cdot g(x'_1)]$$

$$x_1^{*'''} = \operatorname{argmax}_{x''_1} \max_{x_3} [f_3(x''_1, x_3) / g(x''_1)]$$

$$x_1^* = x_1^{*''} = x_1^{*'''}$$



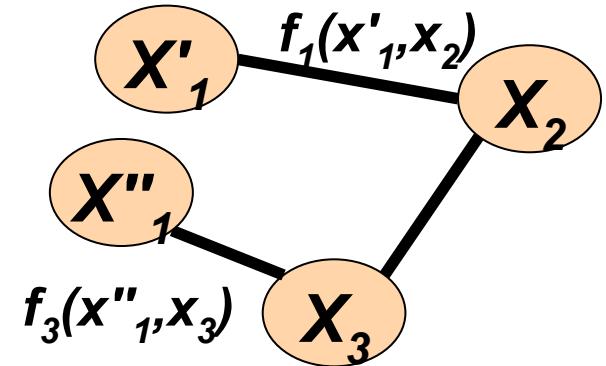
$$\max_{x_2} f_1(x_1, x_2)g(x_1) = \max_{x_3} f_3(x_1, x_3)/g(x_1)$$



# Intuition behind MBE-MM

$$F'_1(x_1, x_2) = f_1(x_1, x_2) \sqrt{\frac{\max_{x_3} f_3(x_1, x_3)}{\frac{\max_{x_2} f_1(x_1, x_2)}{\max_{x_3} f_3(x_1, x_3)}}}$$

$$F''_1(x_1, x_3) = f_3(x_1, x_3) \sqrt{\frac{\max_{x_2} f_1(x_1, x_2)}{\frac{\max_{x_3} f_3(x_1, x_3)}{\max_{x_2} f_1(x_1, x_2)}}}$$



# Linear relaxation-based schemes (MPLP class, Globerson and Jakkola)

**Find:**  $x = (x_1, \dots, x_n)$  to all the variables which maximizes the sum of the factors:

$$\text{MAP}(\theta) = \max_{\mathbf{x}} \sum_{i \in V} \theta_i(x_i) + \sum_{f \in F} \theta_f(\mathbf{x}_f). \quad (1.1)$$

**Best upper bound by Equivalence preserving transformations:**

$$\min_{\delta} L(\delta), \quad (1.2)$$

$$L(\delta) = \sum_{i \in V} \max_{x_i} \left( \theta_i(x_i) + \sum_{f:i \in f} \delta_{fi}(x_i) \right) + \sum_{f \in F} \max_{\mathbf{x}_f} \left( \theta_f(\mathbf{x}_f) - \sum_{i \in f} \delta_{fi}(x_i) \right).$$

$\delta_{fi}(x_i)$  **Is the cost shifted from  $f$  to value  $x_i$  of  $X_i$ .**

**There are several variations of scheme computing the optimizing shifts based on partial gradient descent, which differ by what is being kept constant. The 1.2 task Dual of a linear relaxation of the original problem.**



## Grids

**The dash '-' indicates that the was no solution within 24 hours**

**Time in seconds for grid instances**

**All grids are binary**



Instances (n,w,h)	AOBB-MBE(z) AOBB-MBE-MM(z) AOBB-MPLP(z) z-bound=10	AOBB-MBE(z) AOBB-MBE-MM(z) AOBB-MPLP(z) z-bound=5	AOBB-MBE(z) AOBB-MBE-MM(z) AOBB-MPLP(z) z-bound=3
	time	time	time
50-12-5	0	2	9
144,15,48	0	0	1
	0	1	0
50-14-5	1	64	211
196,18,64	0	6	25
	0	6	24
50-15-5	1	42	431
225,19,76	0	22	24
	0	29	24
50-16-5	97	6759	14047
256,21,79	1	257	11918
	1	209	11872
50-17-5	18	2674	19951
289,22,84	0	70	2293
	0	44	2302
50-18-5	1131	—	—
324,24,84	10	47196	—
	10	19697	—
50-19-5	4664	—	—
361,25,93	9	8808	—
	11	5375	864000
50-20-5	3589	—	—
400,27,97	11	28985	—
	26	6529	—
75-16-5	7	245	2457
256,21,73	0	32	511
	1	37	521
75-17-5	8	279	568
289,22,78	1	186	292
	1	133	301

**The dash '-' indicates that the was no solution within 24 hours**

**Time in seconds for grid instances**

**All grids are binary**



Instances (n,w,h)	AOBB-MBE(z) AOBB-MBE-MM(z) AOBB-MPLP(z) z-bound=10 time	AOBB-MBE(z) AOBB-MBE-MM(z) AOBB-MPLP(z) z-bound=5 time	AOBB-MBE(z) AOBB-MBE-MM(z) AOBB-MPLP(z) z-bound=3 time
90-20-5	14	1199	7281
400,27,99	1 0.9	585 389	5575 5317
90-21-5	15	1585	7722
441,28,106	0 1	861 593	9064 9054
90-22-5	50	2327	27283
484,30,109	6 1	1172 604	17130 17060
90-23-5	564	70188	—
529,31,116	10 17	29635 25511	— —
90-24-5	2393	—	—
576,33,110	73 68	— 27818	— —
90-25-5	2496	—	—
625,34,132	223 277	— —	— —
90-26-5	386	36469	—
676,36,136	21 16	7077 4000	70798 70290
90-30-5	—	—	—
900,42,151	25439 21895	— —	— —

## Runtime for pedigree instances for AOBB

Instances (n,k,w,h)	AOBB-MBE(z) AOBB-MBE-MM(z) AOBB-MPLP(z) z-bound=10	AOBB-MBE(z) AOBB-MBE-MM(z) OBB-MPLP(z) z-bound=8	AOBB-MBE(z) AOBB-MBE-MM(z) OBB-MPLP(z) z-bound=6	AOBB-MBE(z) AOBB-MBE-MM(z) OBB-MPLP(z) z-bound=4
pedigree1 298,4,15,48	0 1 4	1 0 7	0 0 11	0 0 42
pedigree13 88,3,32,102	— 57583 70328	— — —	— — —	— — —
pedigree19 693,5,26,95	— — —	— — —	— — —	— — —
pedigree20 387,5,22,60	44 25 87	137 112 262	167 378 582	4460 10805 11203
pedigree23 309,5,25,51	4 0 9	13 2 24	22 3 20	45 31 89
pedigree25 993,5,25,69	58 0 1	145 4 3	1303 36 48	— 13321 4670
pedigree30 1015,5,21,108	109 21 34	246 36 99	1690 442 508	13198 — —
pedigree31 1006,5,30,85	— — —	— — —	— — —	— — —



*The dash '-' indicates that there was no solution within 24 hours*

## Runtimes for pedigree instances for AOBB

Instances (n,k,w,h)	AOBB-MBE(z) AOBB-MBE-MM(z) AOBB-MPLP(z) z-bound=10	AOBB-MBE(z) AOBB-MBE-MM(z) OBB-MPLP(z) z-bound=8	AOBB-MBE(z) AOBB-MBE-MM(z) OBB-MPLP(z) z-bound=6	AOBB-MBE(z) AOBB-MBE-MM(z) OBB-MPLP(z) z-bound=4
pedigree33 581,4,28,98	89 5 8	177 7 8	201 260 287	24142 1958 2076
pedigree37 726,5,21,56	6 1 0	13 0 1	33 8 6	298 174 145
pedigree39 953,5,21,76	136 15 17	732 29 26	2871 294 377	30724 8315 9100
pedigree50 478,6,17,47	6 17 46	16 11 886	39 47 12146	25440 — —
pedigree51 871,5,39,98	— — —	— — —	— — —	— — —
pedigree7 867,4,32,90	— 1987 4975	— 5993 13211	— 46261 54000	— — —
pedigree9 935,7,27,100	46434 1206 2161	— 7086 9397	— — —	— — —



The dash '-' indicates that there was no solution within 24 hours

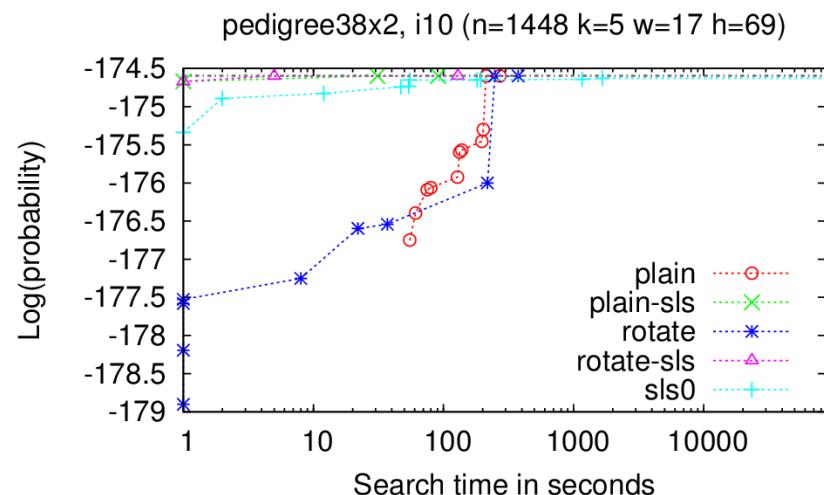
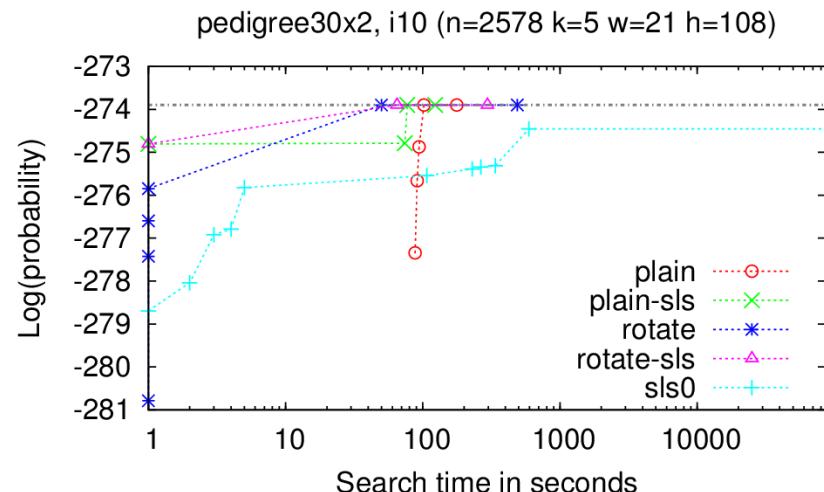
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- Anytime behavior of AOBB (Otten and Dechter, SOCS 2011)
- Improving treewidth (Kask et. Al. 2011)
- Improving mini-bucket partitioning (Rollon 2010)



# Select Anytime Results

- AOBB+SLS receives initial boost
- AOBB+SLS gets to optimality faster

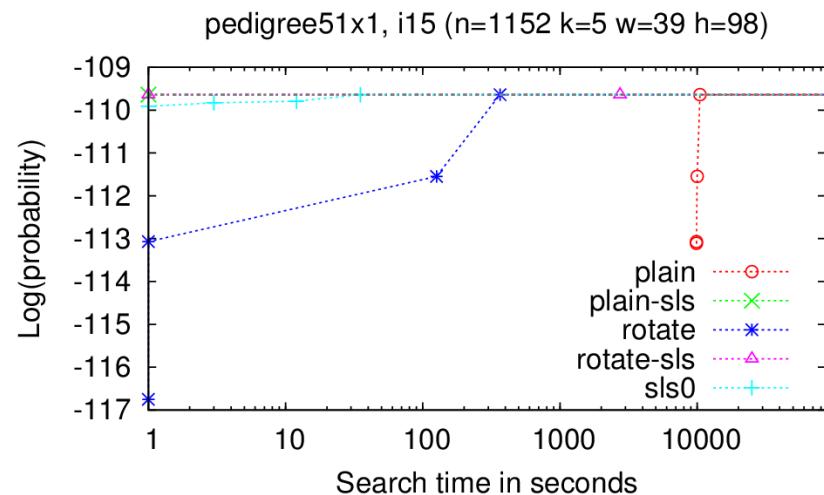
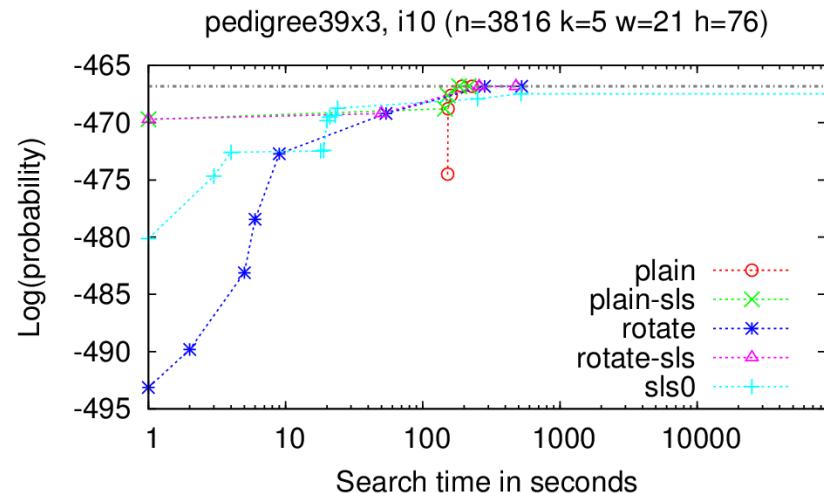


# Select Detailed Results

- AOBB+SLS finds optimal solution, SLS doesn't

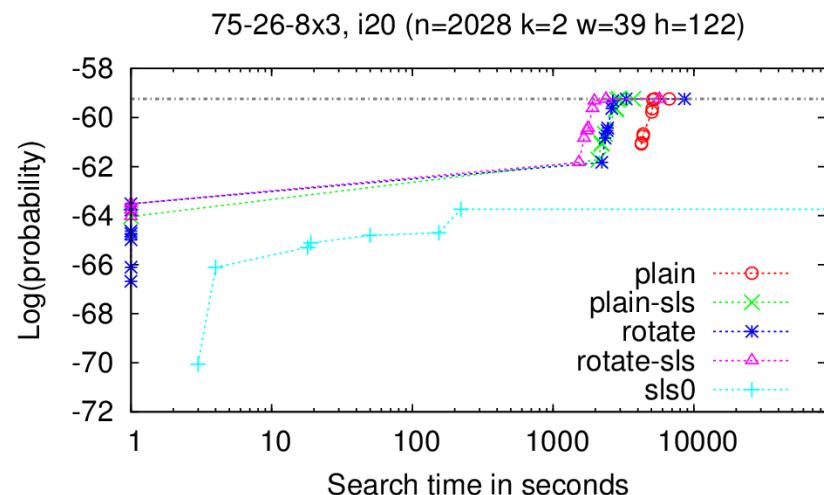
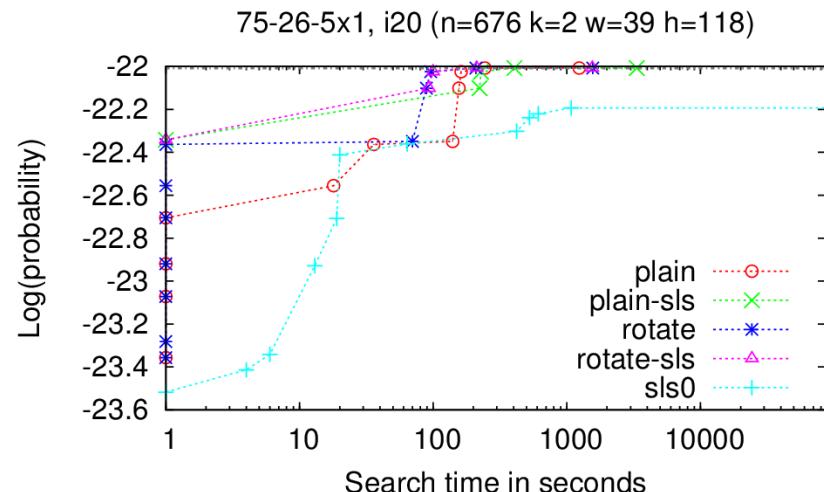


- AOBB+SLS finds optimum right away



# Select Detailed Results

- All AOBB variants outperform SLS, reach optimality
- Rotating AOBB receives boost from initial SLS



# Software

- AND/OR search algorithms
- Bucket-tree elimination
- Generalized belief propagation
- Samplesearch sampling

are available at:

<http://graphmod.ics.uci.edu/group/Software>



**Thank you!**

