

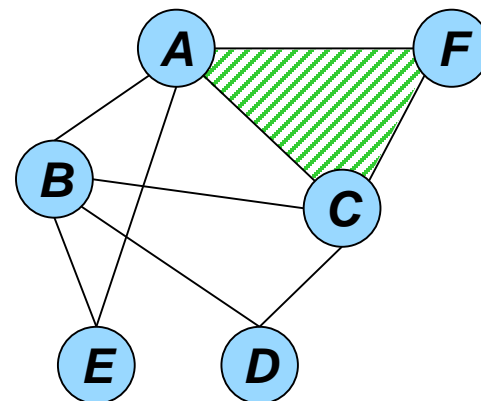
# Modern Exact and Approximate Combinatorial Optimization algorithms for Graphical Models

*In the pursuit of a universal solver*

**Rina Dechter**

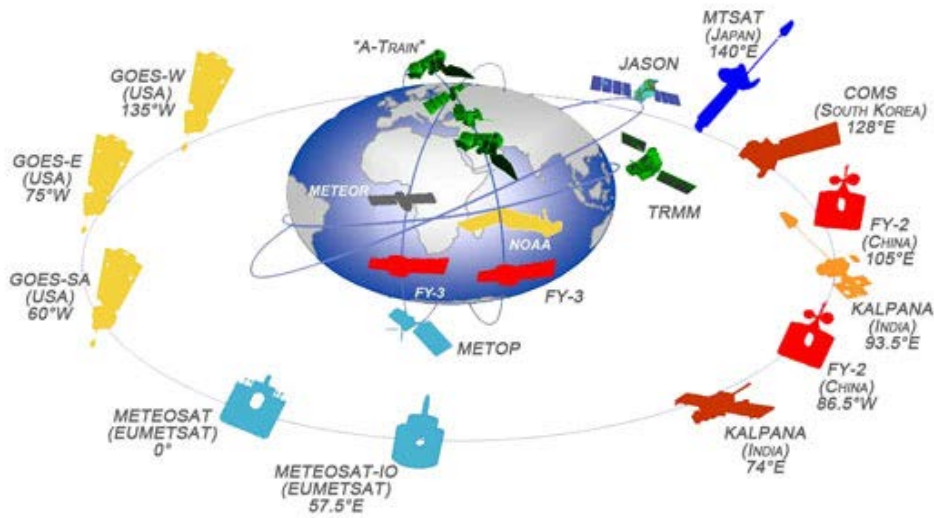
Donald Bren school of ICS, University of California, Irvine

*Main collaborator:*  
*Radu Marinescu*  
*Lars Otten*  
*Alex Ihler*  
*Kalev Kask*  
*Robert Mateescu*

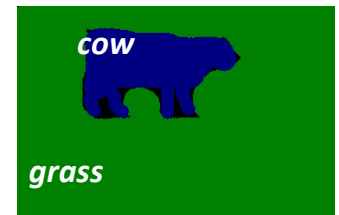
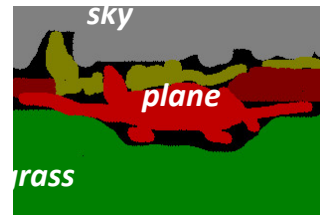


# Combinatorial Optimization

## Planning & Scheduling



## Computer Vision



*Find an optimal schedule for the satellite that maximizes the number of photographs taken, subject to on-board recording capacity*

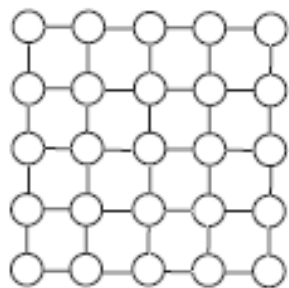
*Image classification: label pixels in an image by their associated object class*

*[He et al. 2004; Winn et al. 2005]*

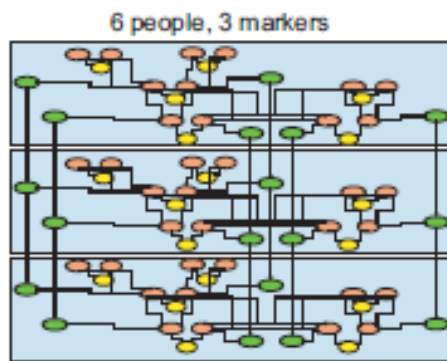
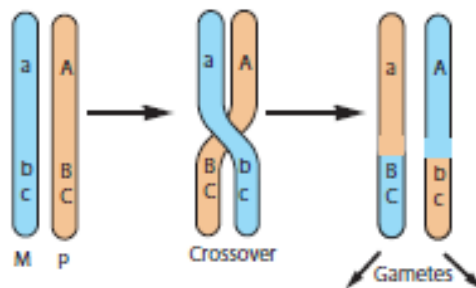


# Sample Applications for Graphical Models

## Computer Vision



## Genetic Linkage



## Sensor Networks



Figure 1: Application areas and graphical models used to represent their respective systems: (a) Finding correspondences between images, including depth estimation from stereo; (b) Genetic linkage analysis and pedigree data; (c) Understanding patterns of behavior in sensor measurements using spatio-temporal models.



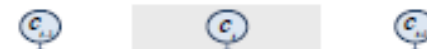
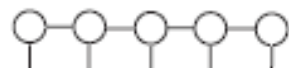
# Sample Applications for Graphical Models

Computer Vision

Genetic Linkage

Sensor Networks

***Learning: MAP***



***Reasoning: MAP***

Figure 1: Application areas and graphical models used to represent their respective systems: (a) Finding correspondences between images, including depth estimation from stereo; (b) Genetic linkage analysis and pedigree data; (c) Understanding patterns of behavior in sensor measurements using spatio-temporal models.



# How to Design a Good MAP Solver

- Heuristic Search
- The core of a good search algorithm
  - A compact search space
  - A good heuristic evaluation function
  - A good traversal strategy
- Anytime search yields a good approximation.



# Outline

- Graphical models, Queries, Algorithms
- Inference Algorithms: bucket-elimination
- Bounded Inference: a) mini-bucket, b) cost-shifting
- AND/OR search spaces and AND/OR BnB
- Evaluation, Software
- Conclusion



# ***Graphical Models, Queries, Algorithms***

***Any collection of local functions over a subset of variable  
Is a graphical model***



# 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	0
2	3	1	0
3	1	2	5
3	2	1	0

*Primal graph =*

*Variables --> nodes*

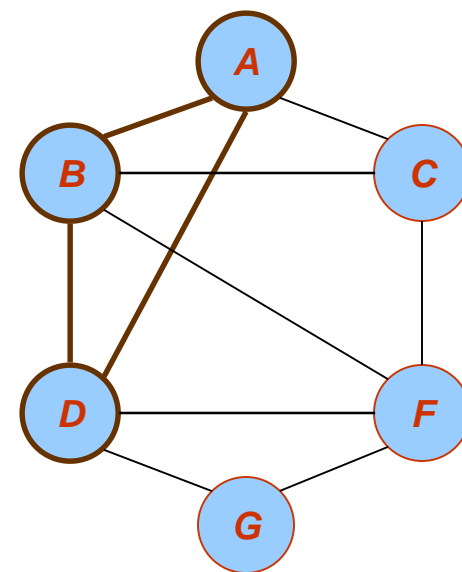
*Functions, Constraints -> arcs*

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

Global Cost Function

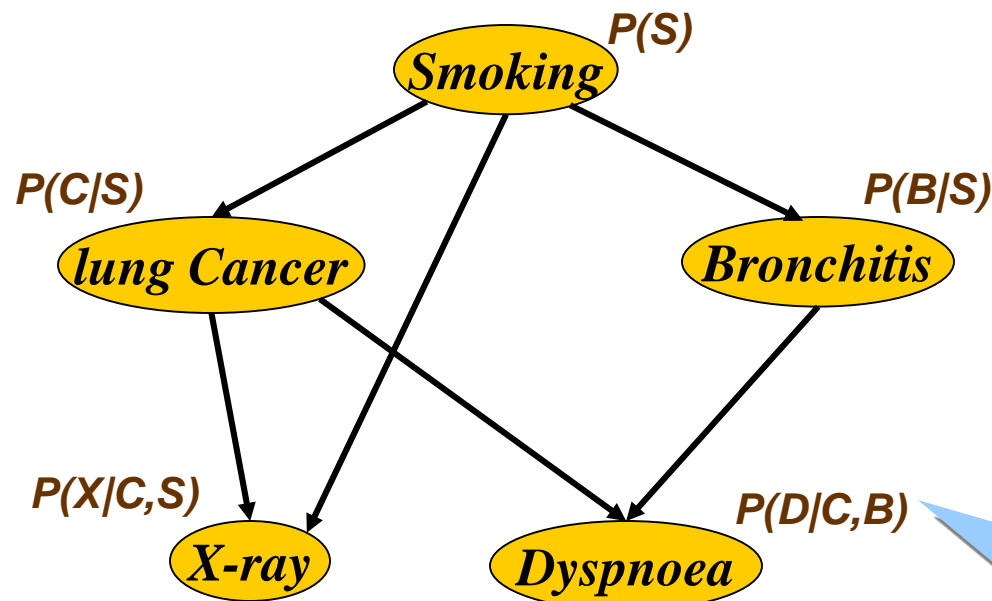
$$F(X) = \sum_{i=1}^m f_i(X)$$

CMU 2016





# Bayesian Networks (Pearl, 1988)



**BN = (G, Θ)**

**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

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

**Belief Updating:**

**$P(\text{lung cancer}=\text{yes} \mid \text{smoking}=\text{no}, \text{dyspnoea}=\text{yes}) = ?$**

**MPE = find argmax  $P(S) \cdot P(C|S) \cdot P(B|S) \cdot P(X|C,S) \cdot P(D|C,B)$**



# Graphical Models

■ A graphical model  $(\mathbf{X}, \mathbf{D}, \mathbf{F})$ :

- $\mathbf{X} = \{X_1, \dots, X_n\}$  variables
- $\mathbf{D} = \{D_1, \dots, D_n\}$  domains
- $\mathbf{F} = \{f_1, \dots, f_r\}$  functions  
(constraints, CPTs, CNFs ...)

■ Operators:

- combination : Sum, product, join
- Elimination: projection, sum, max/min

■ Tasks:

- **Belief updating:**  $\sum_{X \setminus Y} \prod_j P_j$
- **MPE \ MAP:**  $\max_X \prod_j P_j$
- **Marginal MAP:**  $\max_Y \sum_{X \setminus Y} \prod_j P_j$

□ **CSP:**  $\prod_{X \times_j} C_j$

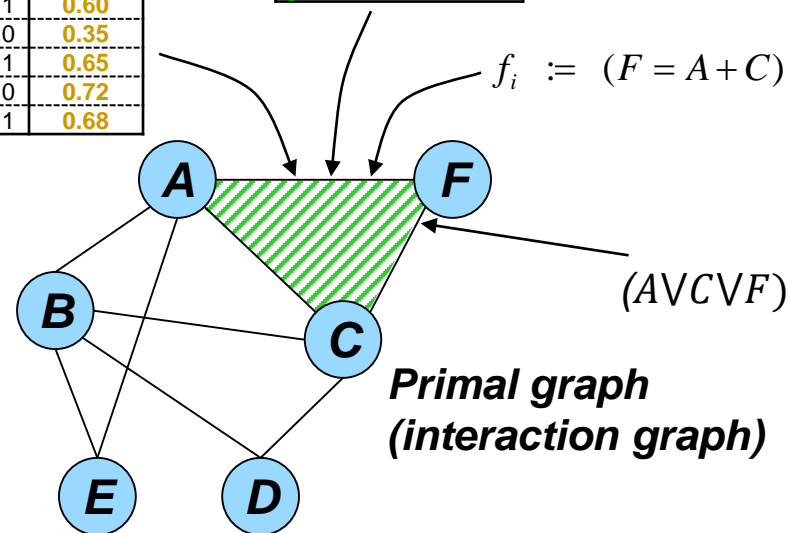
□ **Max-CSP:**  $\min_X \sum_j F_j$

**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



**All these tasks are NP-hard**

- exploit problem structure
- identify special cases
- approximate

# Example Domains for Graphical Models

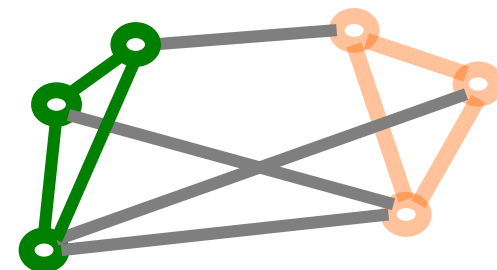
- Natural Language Processing
  - Information extraction, semantic parsing, translation, summarization, ...
- Computer Vision
  - Object recognition, scene analysis, segmentation, tracking, ...
- Computational Biology
  - Pedigree analysis, protein folding / binding / design, sequence matching, ...
- Networks
  - Webpage link analysis, social networks, communications, citations, ...
- Robotics
  - Planning & decision making, ...



# Max-product = min-sum

*max (A,B)*

$$x_{AB}^* = \arg \max_{x_A, x_B} \prod_{x_\alpha} \varphi_\alpha$$



$$x_{AB}^* = \arg \min_{x_A, x_B} \sum_{x_\alpha} \varphi'_\alpha$$

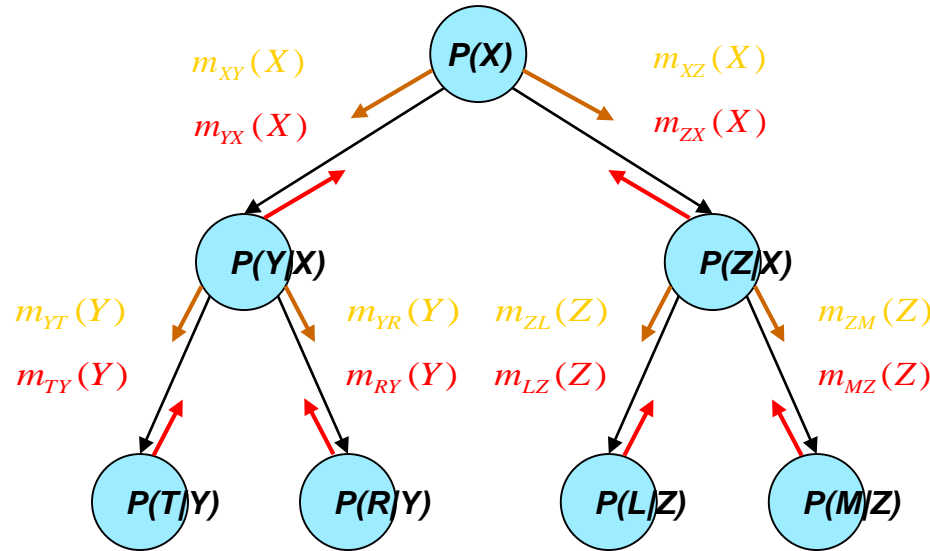
$$\varphi'_\alpha = -\log \varphi_\alpha$$



# Tree-solving is easy

*Belief updating  
(sum-prod)*

*CSP – consistency  
(projection-join)*



*MPE (max-prod)*

*#CSP (sum-prod)*

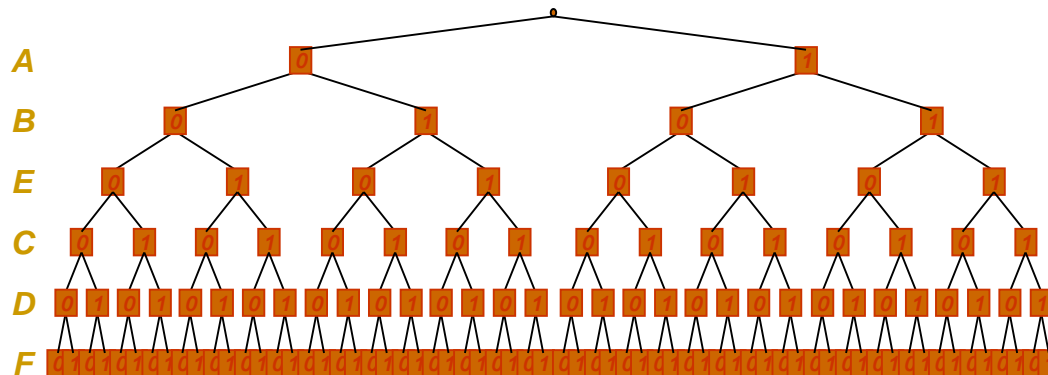
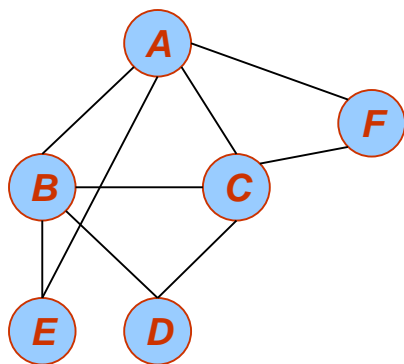
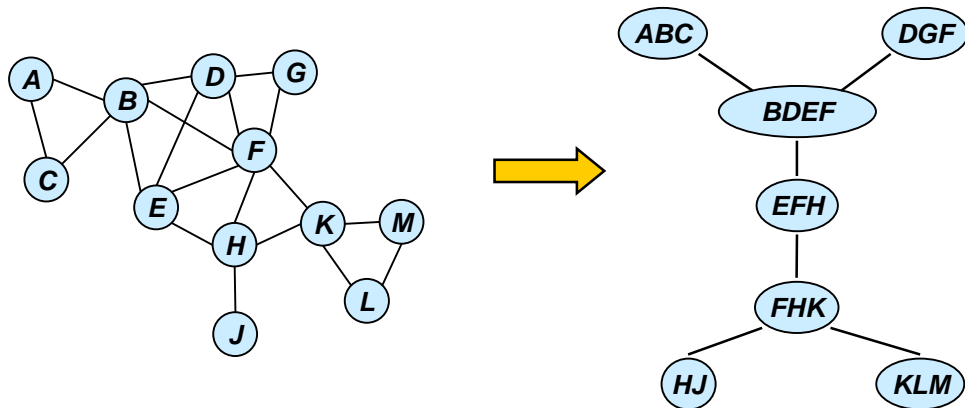
**Trees are processed in linear time and memory**



# Inference vs conditioning-search

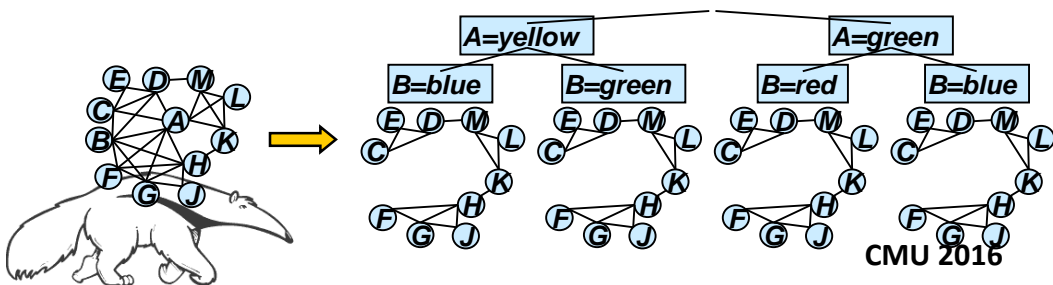
## *Inference*

*exp(w\*) time/space*



## *Search*

*Exp(n) time*  
*O(n) space*



**Search+inference:**

**Space:  $exp(w)$**

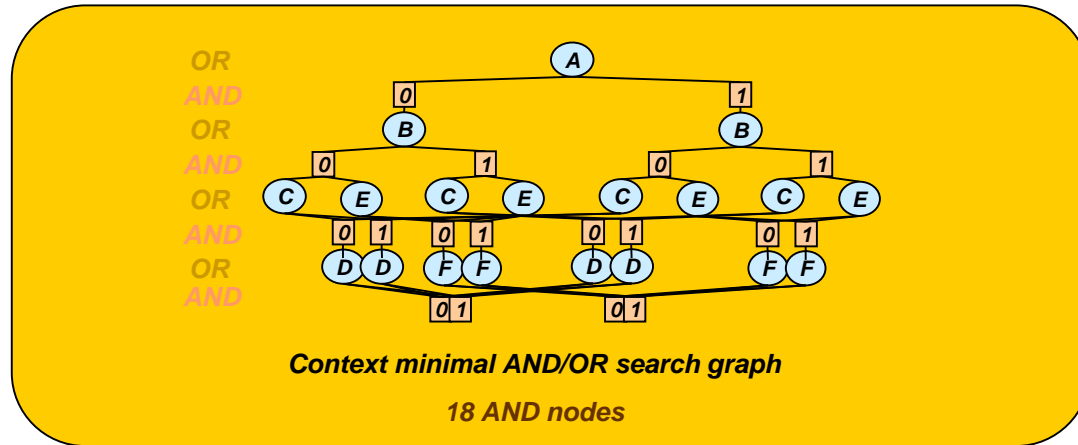
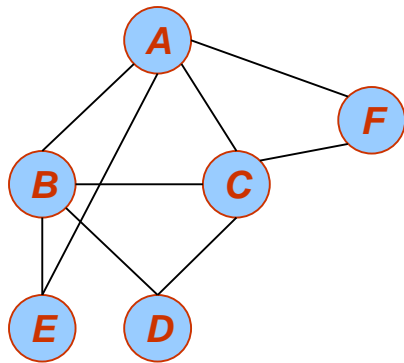
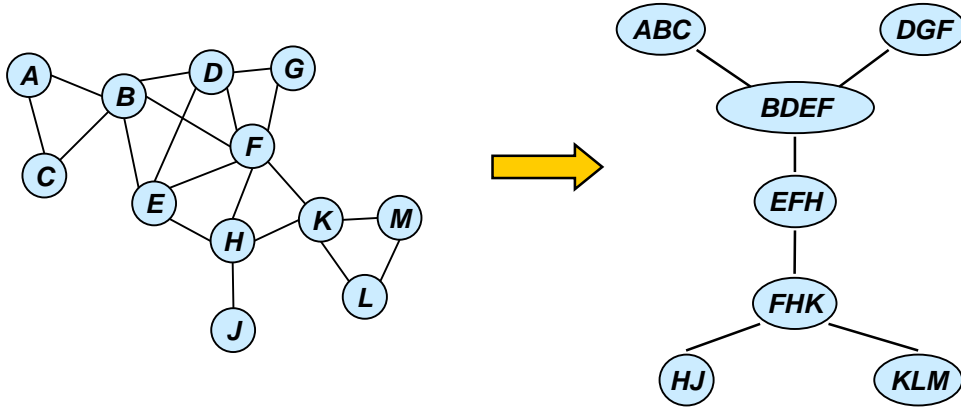
**Time:  $exp(w+c(w))$**

*w: user controlled*

# Inference vs conditioning-search

## *Inference*

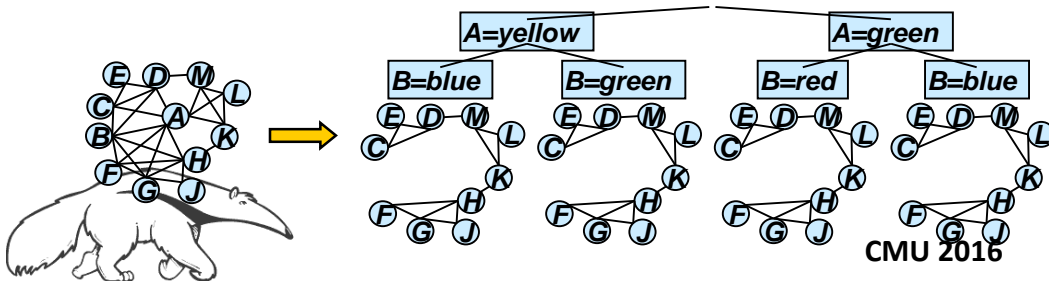
*exp(w\*) time/space*



## *Search*

*Exp(w\*) time*

*O(w\*) space*



**Search+inference:**

**Space:  $exp(q)$**

**Time:  $exp(q+c(q))$**

**q: user controlled**

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- Graphical models, Queries, Algorithms
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- Evaluation, Software
- Conclusions

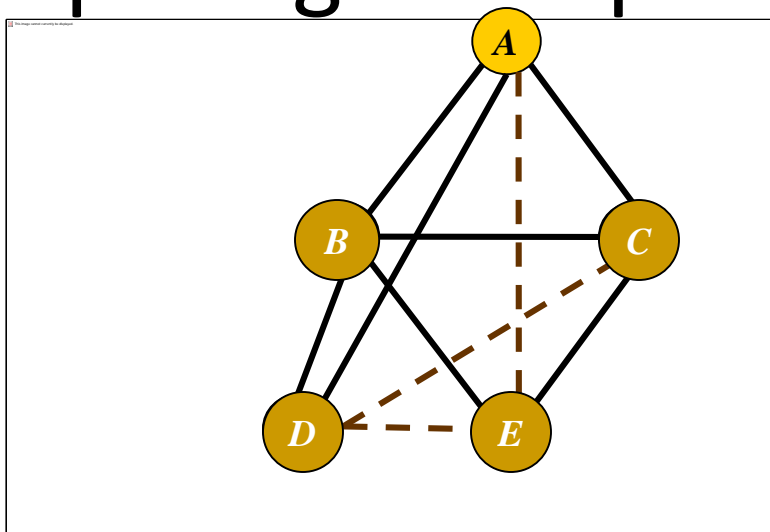




- ***Solving MAP by Inference:***
- ***Non-serial Dynamic programming***
- ***The induced-width/treewidth***



# Computing the Optimal Cost Solution



$$OPT = \min_{e=0,d,c,b} \underbrace{f(a,b)+f(a,c)+f(a,d)} + \underbrace{f(b,c)+f(b,d)+f(b,e)+f(c,e)}$$

**Combination**

$$\min_{e=0} \min_d f(a,d) + \min_c f(a,c)+f(c,e) + \min_b \underbrace{f(a,b)+f(b,c)+f(b,d)+f(b,e)}_{\lambda_{B \rightarrow C}(a,d,c,e)}$$

**Variable Elimination**



# Bucket Elimination

Algorithm *elim-opt* [Dechter, 1996]

Non-serial Dynamic Programming [Bertele & Briochi, 1973]

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

$$\min_b \sum \leftarrow \text{Elimination/Combination operators}$$

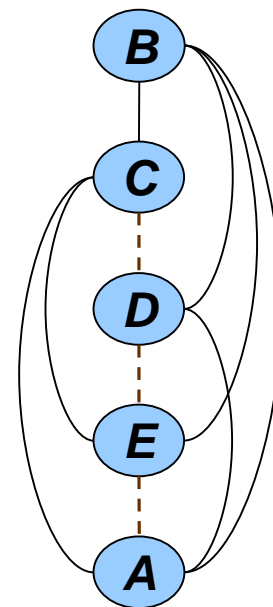
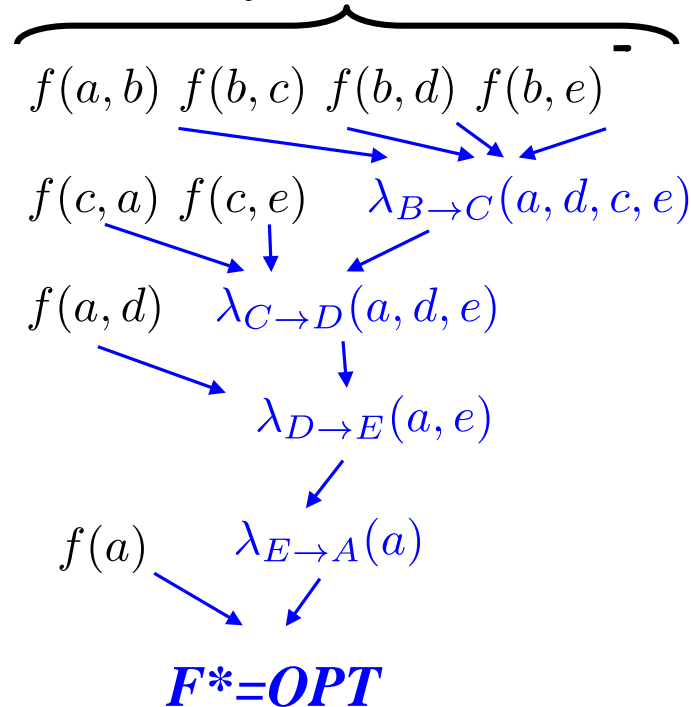
**bucket B:**

**bucket C:**

**bucket D:**

**bucket E:**

**bucket A:**



# Complexity of Bucket Elimination

Algorithm elim-opt [Dechter, 1996]

Non-serial Dynamic Programming [Bertele & Briochi, 1973]

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

$$\min_b \sum \leftarrow \text{Elimination/Combination operators}$$

**bucket B:**

$$f(a,b) \quad f(b,c) \quad f(b,d) \quad f(b,e)$$

**bucket C:**

$$f(c,a) \quad f(c,e) \quad \lambda_{B \rightarrow C}(a, d, c, e)$$

**bucket D:**

$$f(a,d) \quad \lambda_{C \rightarrow D}(a, d, e)$$

**bucket E:**

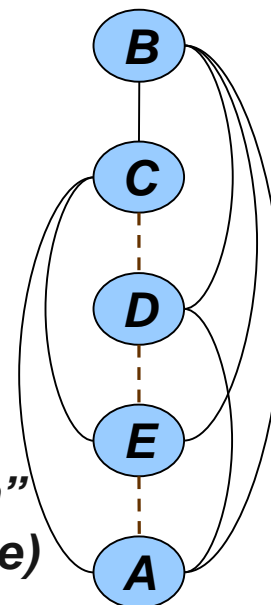
$$\lambda_{D \rightarrow E}(a, e)$$

**bucket A:**

$$f(a) \quad \lambda_{E \rightarrow A}(a)$$

$$F^* = OPT$$

$\exp(w^*=4)$   
"induced width"  
(max clique size)



# Generating the Optimal Assignment

$$b^* = \arg \min_b f(a^*, b) + f(b, c^*) \\ + f(b, d^*) + f(b, e^*)$$

**B:**  $f(a, b) \ f(b, c) \ f(b, d) \ f(b, e)$

***Time and space exponential in the induced-width / treewidth***

$$O(nk^{w^*+1})$$

**Return:**  $(a^*, b^*, c^*, d^*, e^*)$



# Complexity of Bucket Elimination

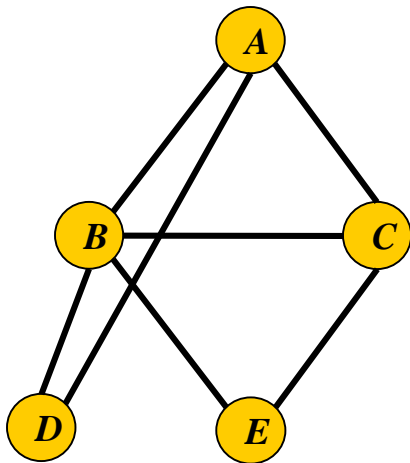
**Bucket Elimination is time and space**

$$O(r \exp(w^*(d)))$$

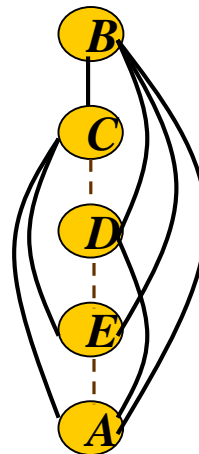
$w^*(d)$  – the induced width of graph along ordering  $d$

$r$  = number of functions

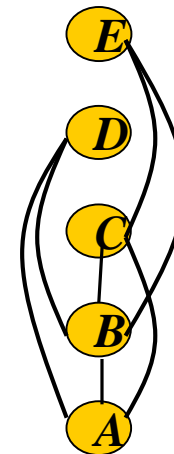
*The effect of the ordering:*



“Moral” graph



$$w^*(d_1) = 4$$



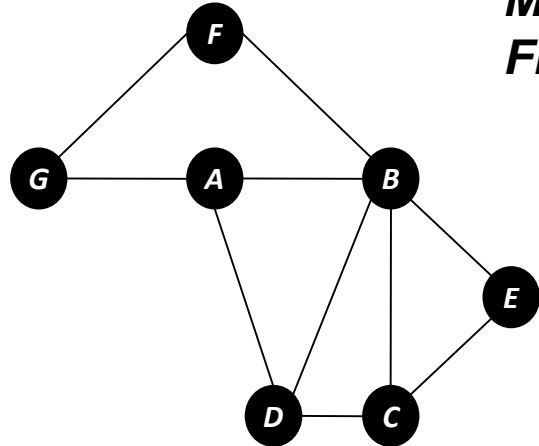
$$w^*(d_2) = 2$$



**Finding the smallest induced width is hard!**

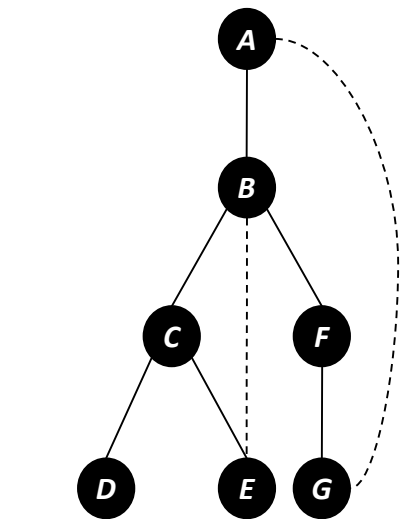
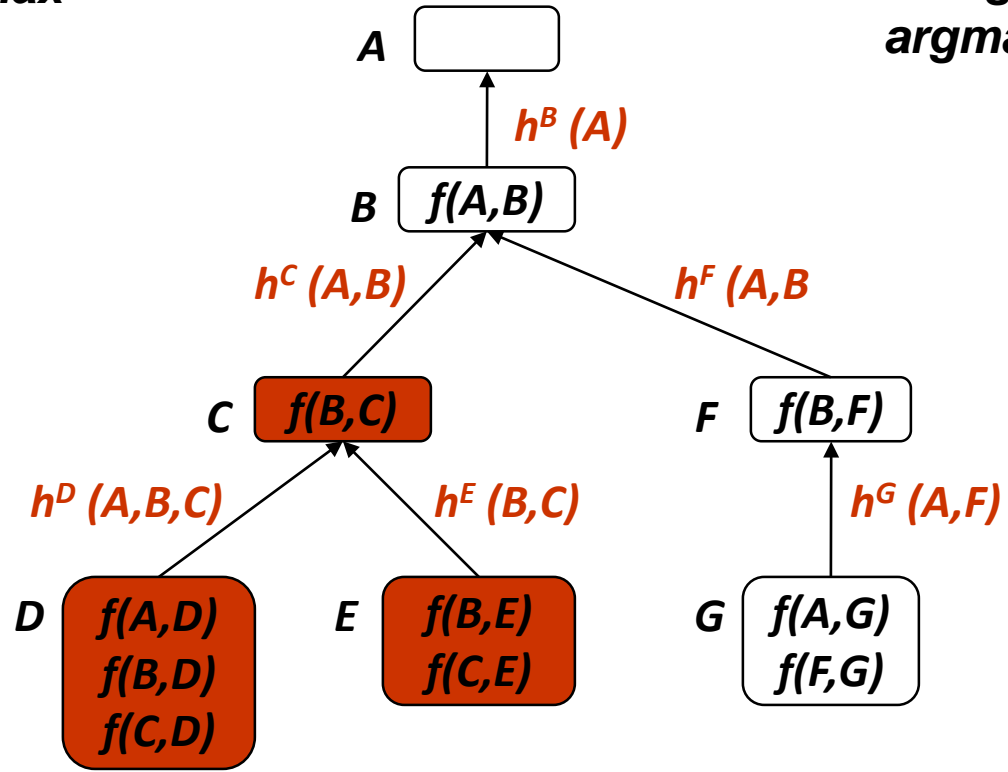
# Bucket Elimination

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



**Messages**  
*Finding max*

**Assignment**  
*argmax*



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



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- AND/OR search spaces and AND/OR BnB
- Evaluation, Software
- Conclusions





# Bounding approximations: Generating a heuristic evaluation function

- ***The mini-bucket scheme***
- *The cost-shifting or re-parameterization scheme*
- *Combining the two*



# Mini-Bucket Approximation

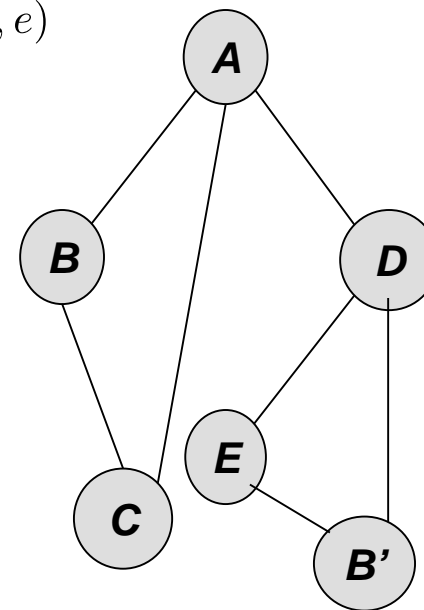
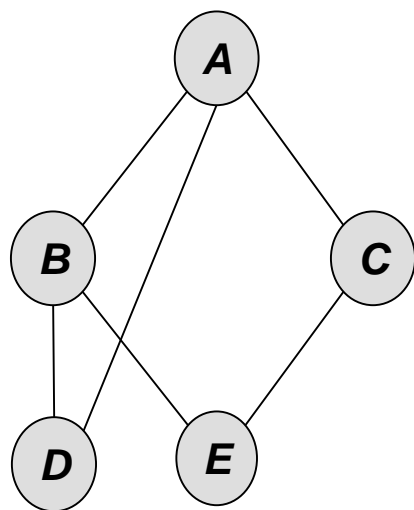
*Split a bucket into mini-buckets => bound complexity*

$$\begin{aligned}
 & \mathbf{bucket}(X) = \\
 & \{ f_1, \dots, f_r, f_{r+1}, \dots, f_n \} \\
 & \underbrace{\hspace{10em}} \\
 & \swarrow \hspace{2em} \lambda_X(\cdot) = \min_x \sum_{i=1}^n f_i(x, \dots) \hspace{2em} \searrow \\
 & \{ f_1, \dots, f_r \} \hspace{15em} \{ f_{r+1}, \dots, f_n \} \\
 & \lambda'_X(\cdot) = \left( \min_x \sum_{i=1}^r f_i(\cdot) \right) + \left( \min_x \sum_{i=r+1}^n f_i(\cdot) \right) \\
 & \lambda'_X(\cdot) \leq \lambda_X(\cdot)
 \end{aligned}$$

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



# Mini-Bucket Elimination



$$\min_{B'} \sum f(\cdot) \xrightarrow{\text{mini-buckets}} \min_B \sum f(\cdot)$$

**bucket B:**  $f(a, b) \quad f(b, c) \quad f(b, d) \quad f(b, e)$

**bucket C:**  $\lambda_{B \rightarrow C}(a, c) \quad f(a, c) \quad f(c, e)$

**bucket D:**  $f(a, d) \quad \lambda_{B \rightarrow D}(d, e)$

**bucket E:**  $\lambda_{C \rightarrow E}(a, e) \quad \lambda_{D \rightarrow E}(a, e)$

**bucket A:**  $f(a) \quad \lambda_{E \rightarrow A}(a)$

**L = lower bound**

[Dechter and Rish, 1997; 2003]

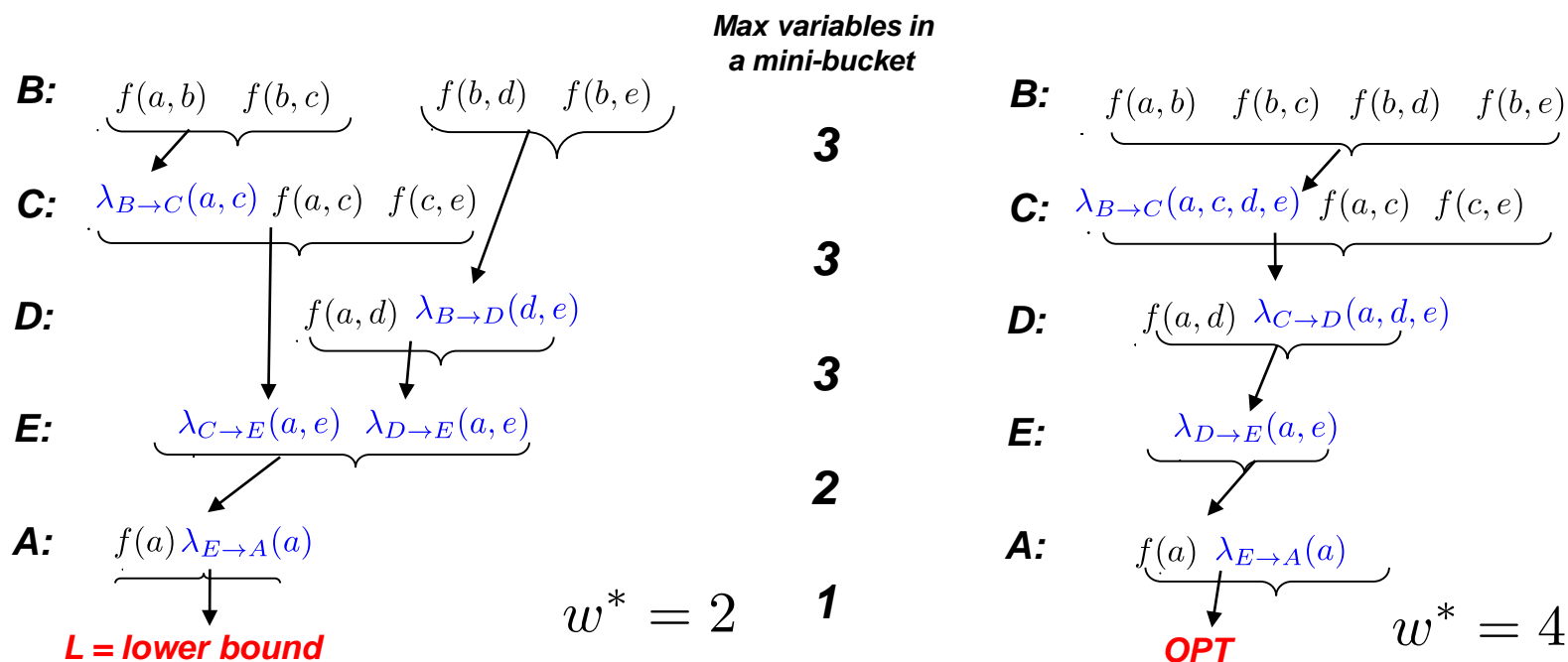
**Model relaxation:**  
[Kask et al., 2001]  
[Geffner et al., 2007]  
[Choi et al., 2007]  
[Johnson et al. 2007]



# MBE-MPE(i) vs BE-MPE

- **Input:**  $i$  – max number of variables allowed in a mini-bucket
- **Output:** [lower bound (P of a suboptimal solution), upper bound]

**MBE-MPE(3)** versus **BE-MPE**



# Mini-Bucket Decoding

$$\mathbf{b}^* = \arg \min_{\mathbf{b}} f(a^*, b) + f(b, c^*) + f(b, d^*) + f(b, e^*)$$

$$\mathbf{c}^* = \arg \min_{\mathbf{c}} f(c, a^*) + f(c, e^*) + \lambda_{B \rightarrow C}(a^*, d^*, c, e^*)$$

$$\mathbf{d}^* = \arg \min_{\mathbf{d}} f(a^*, d) + \lambda_{C \rightarrow D}(a^*, d, e^*)$$

$$\mathbf{e}^* = \arg \min_{\mathbf{e}} \lambda_{D \rightarrow E}(a^*, e)$$

$$\mathbf{a}^* = \arg \min_{\mathbf{a}} f(a) + \lambda_{E \rightarrow A}(a)$$

$$\mathbf{B:} \quad f(a, b) \quad f(b, c) \quad f(b, d) \quad f(b, e)$$

$$\mathbf{C:} \quad f(c, a) \quad f(c, e) \quad \lambda_{B \rightarrow C}(a, d, c, e)$$

$$\mathbf{D:} \quad f(a, d) \quad \lambda_{C \rightarrow D}(a, d, e)$$

$$\mathbf{E:} \quad \lambda_{D \rightarrow E}(a, e)$$

$$\mathbf{A:} \quad f(a) \quad \lambda_{E \rightarrow A}(a)$$

**Return:** (  $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*, \mathbf{d}^*, \mathbf{e}^*$  )

**Greedy configuration = upper bound**

**L = lower bound**



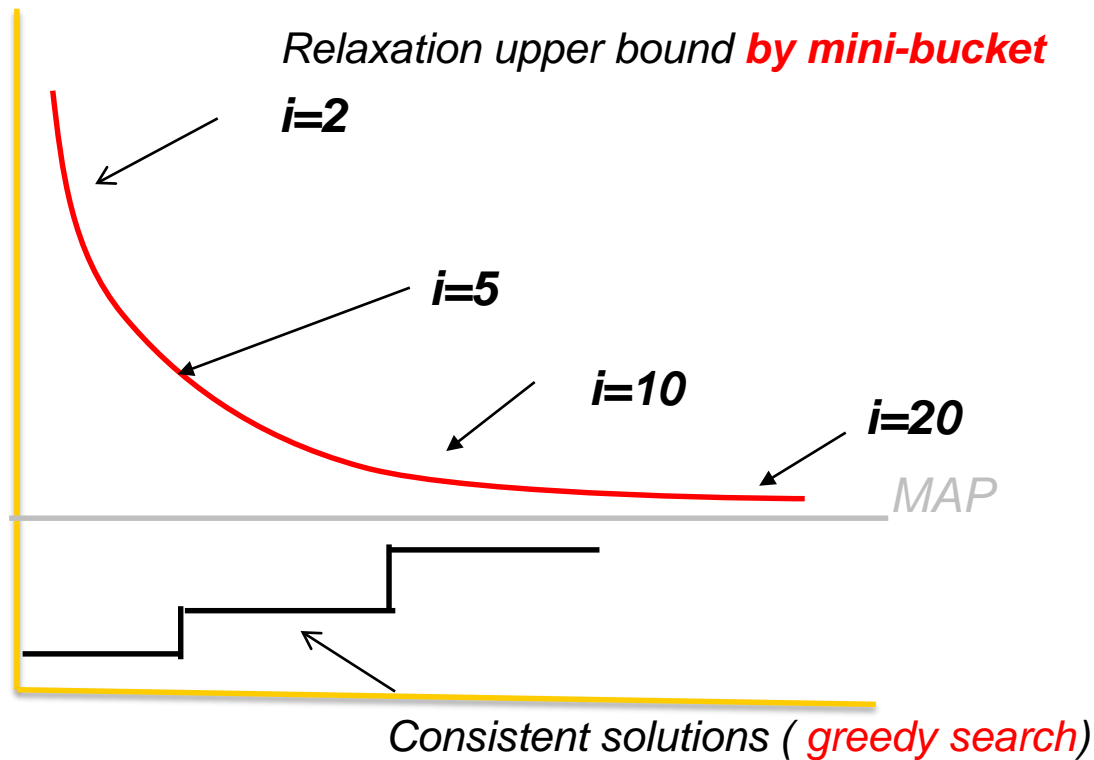
# Properties of MBE(i)

- **Complexity:**  $O(n \exp(i))$  time and  $O(\exp(i))$  space
- Yields a lower bound and an upper bound
- **Accuracy** estimatable by the upper/lower (U/L) bounds
- Possible use of mini-bucket approximations:
  - As **anytime algorithms**
  - As **heuristics** in search
- Other tasks (similar mini-bucket approximations):
  - Belief updating, Marginal MAP, MEU, WCSP, MaxCSP

*[Dechter and Rish, 1997], [Liu and Ihler, 2011], [Liu and Ihler, 2013]*



# Bounding from above and below



How to partition given an i-bound?

- Scope-based greedy
- Content-based greedy
- (Rollon & Dechter 2010)

Relaxation provides upper bound  
Any configuration: lower bound



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# Cost-Shifting

*(Reparameterization)*

$+\lambda(B)$

A	B	f(A,B)
b	b	6 + 3
b	g	0 - 1
g	b	0 + 3
g	g	6 - 1

$-\lambda(B)$

B	C	f(B,C)
b	b	6 - 3
b	g	0 - 3
g	b	0 + 1
g	g	6 + 1

+

A	B	C	f(A,B,C)
b	b	b	12
b	b	g	6
b	g	b	0
b	g	g	6
g	b	b	6
g	b	g	0
g	g	b	6
g	g	g	12

= 0 + 6

*Modify the individual functions*

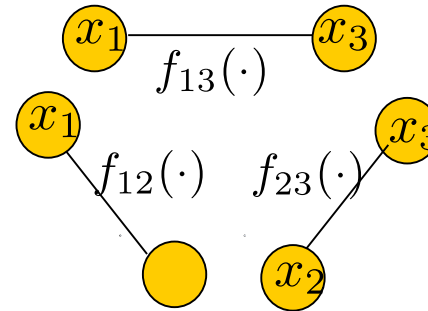
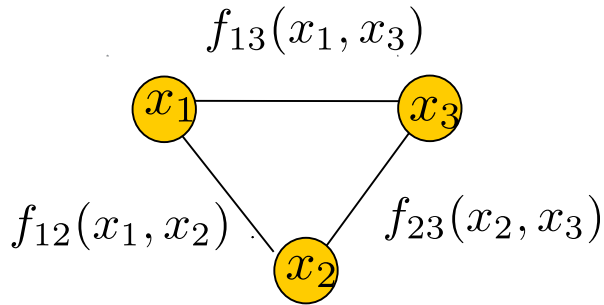
*- but -*

*keep the sum of functions unchanged*

B	$\lambda(B)$
b	3
g	-1



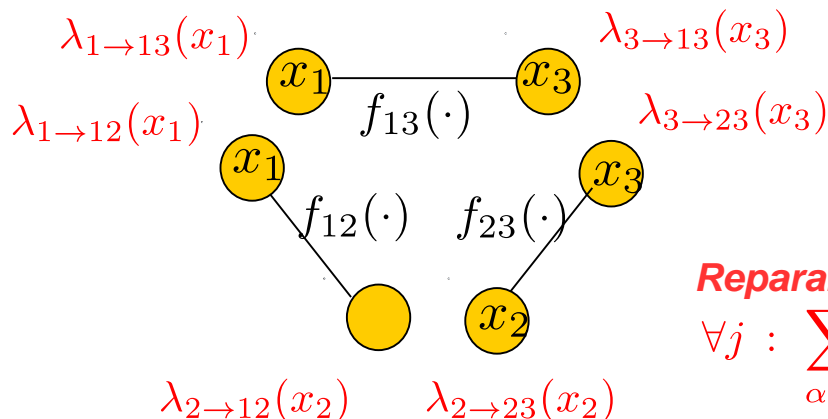
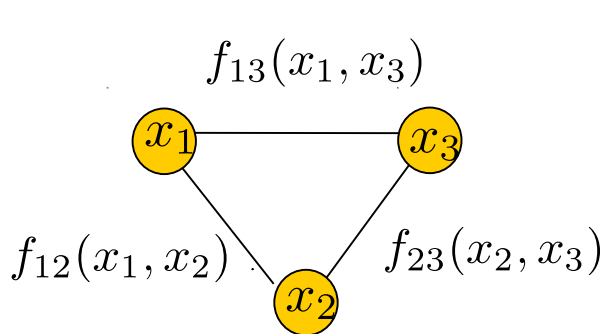
# Dual Decomposition



$$F^* = \min_x \sum_{\alpha} f_{\alpha}(x) \quad \geq \quad \sum_{\alpha} \min_x f_{\alpha}(x)$$



# Dual Decomposition



**Reparameterization:**

$$\forall j : \sum_{\alpha \ni j} \lambda_{j \rightarrow \alpha}(x_j) = 0$$

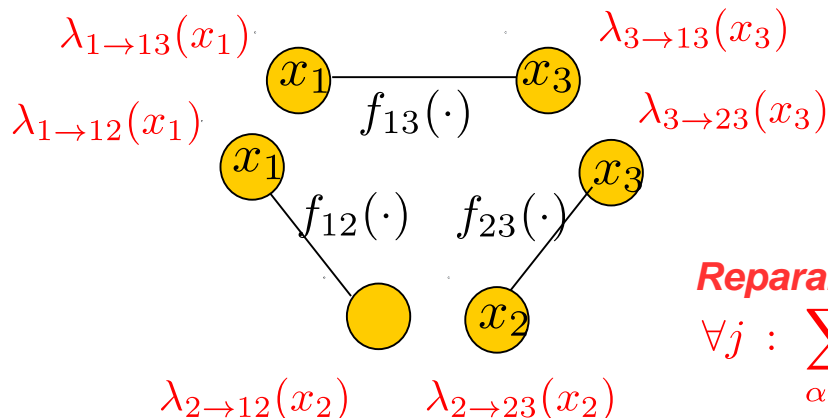
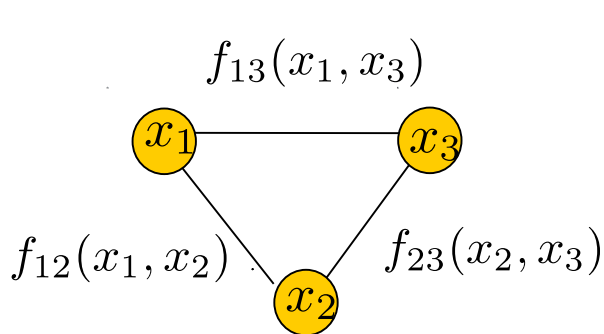
$$F^* = \min_x \sum_{\alpha} f_{\alpha}(x) \geq \max_{\lambda_{i \rightarrow \alpha}} \sum_{\alpha} \min_x \left[ f_{\alpha}(x) + \sum_{i \in \alpha} \lambda_{i \rightarrow \alpha}(x_i) \right]$$

- Bound solution using decomposed optimization
- Solve independently: optimistic bound
- Tighten the bound by reparameterization
  - Enforce lost equality constraints via Lagrange multipliers



(Convex dual: linear programming relaxation)

# Dual Decomposition



**Reparameterization:**  
 $\forall j : \sum_{\alpha \ni j} \lambda_{j \rightarrow \alpha}(x_j) = 0$

$$F^* = \min_x \sum_{\alpha} f_{\alpha}(x) \geq \max_{\lambda_{i \rightarrow \alpha}} \sum_{\alpha} \min_x \left[ f_{\alpha}(x) + \sum_{i \in \alpha} \lambda_{i \rightarrow \alpha}(x_i) \right]$$

Many names for the same class of bounds:

- Dual decomposition [Komodakis et al. 2007]
- TRW, MPLP [Wainwright et al. 2005, Globerson & Jaakkola 2007]
- Soft arc consistency [Cooper & Schiex 2004]
- Max-sum diffusion [Warner 2007]

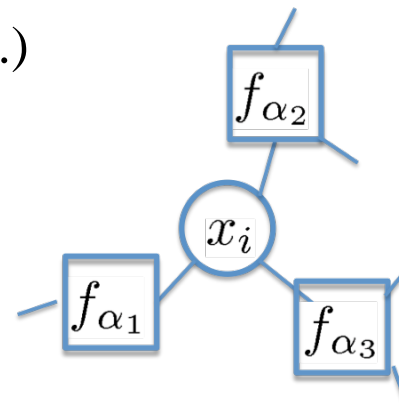


(Convex dual: linear programming relaxation)

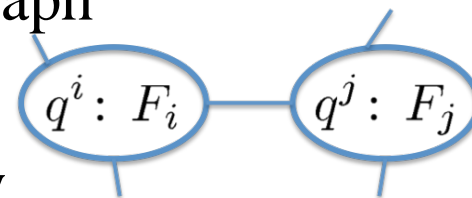
# Various Update Schemes

- Can use any decomposition updates
  - (message passing, subgradient, augmented, etc.)

- **FGLP**: Update the original factors



- **JGLP**: Update clique function of the join graph



- **MBE-MM** Update within each bucket only

- Apply cost-shifting within each bucket only



# Factor graph Linear Programming

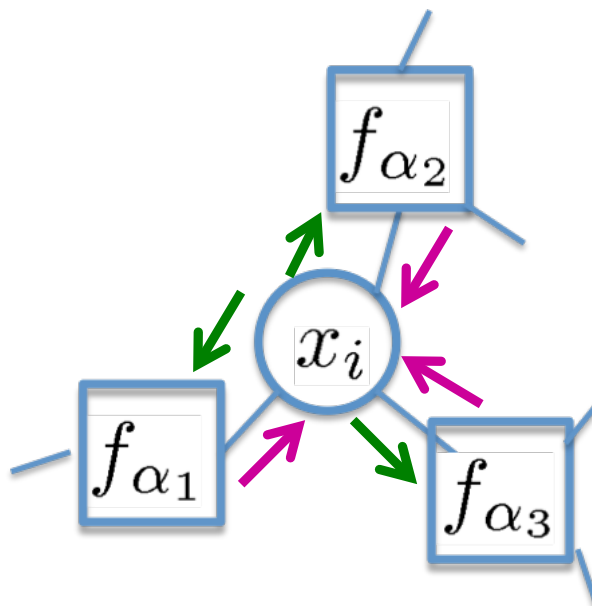
- Update the original factors (FGLP)

- Tighten all factors over  $x_i$  simultaneously

- Compute **max-marginals**  $\forall \alpha, \gamma_\alpha(x_i) = \max_{x_\alpha \setminus x_i} f_\alpha$

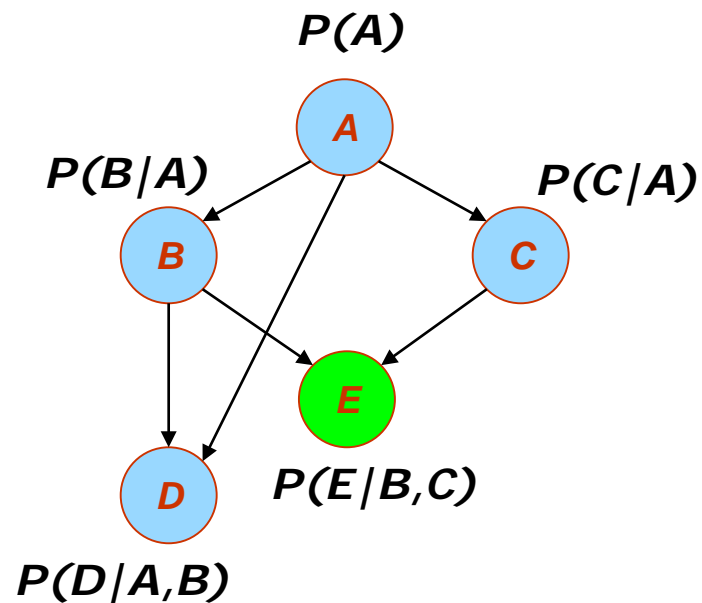
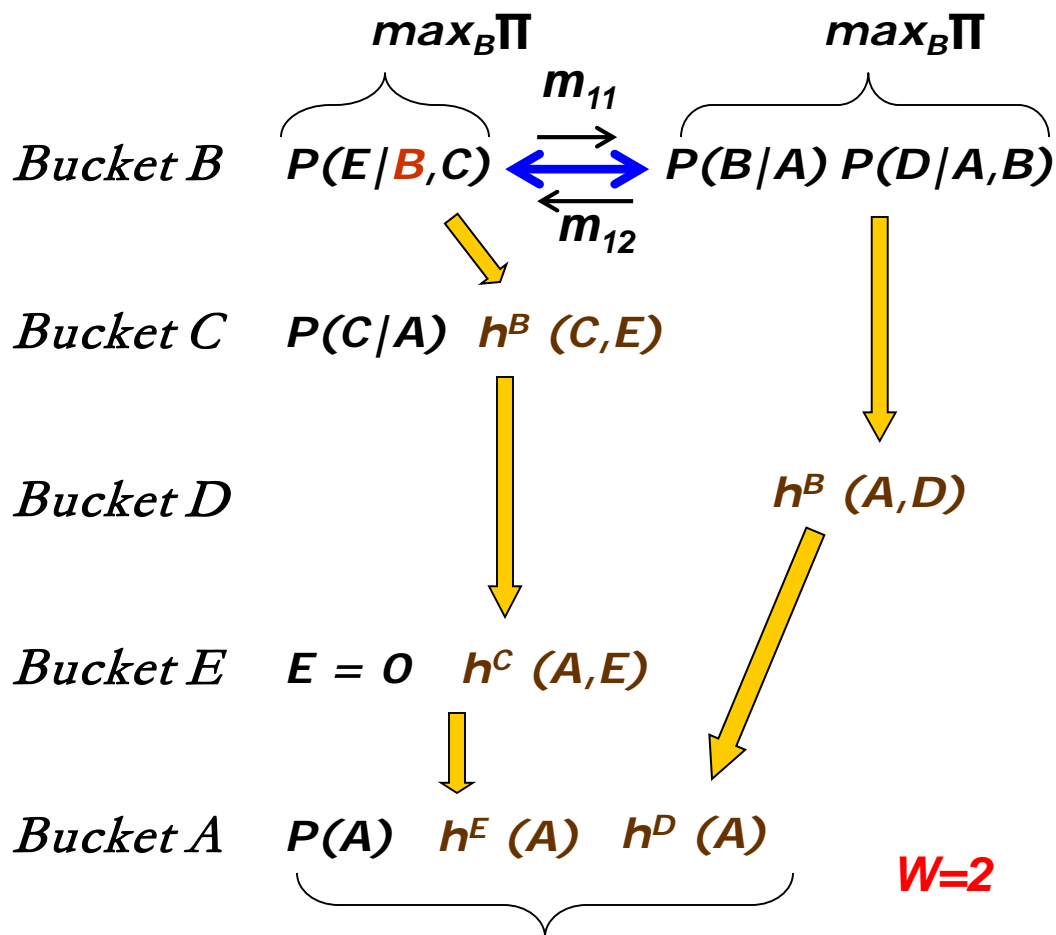
- & **update**:

$$\forall \alpha, f_\alpha(x_\alpha) \leftarrow f_\alpha(x_\alpha) - \gamma_\alpha(x_i) + \frac{1}{|F_i|} \sum_{\beta} \gamma_\beta(x_i)$$



# MBE-MM: MBE with moment matching

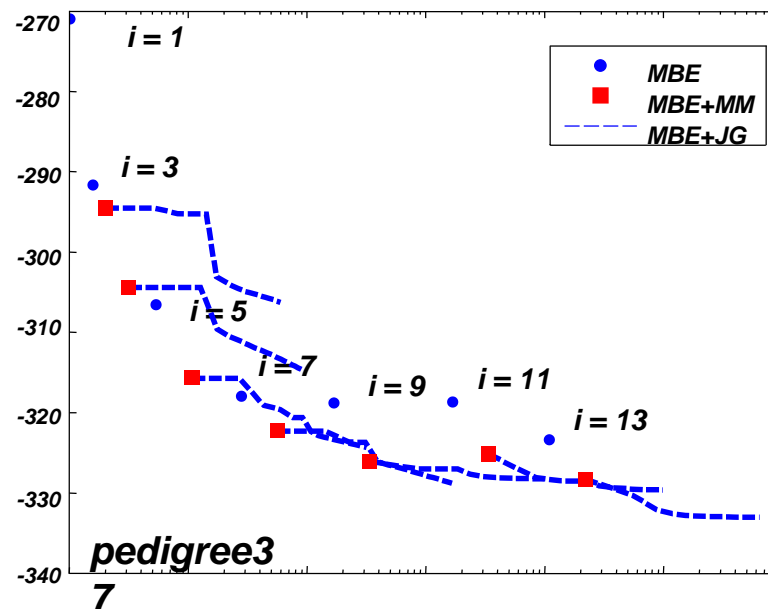
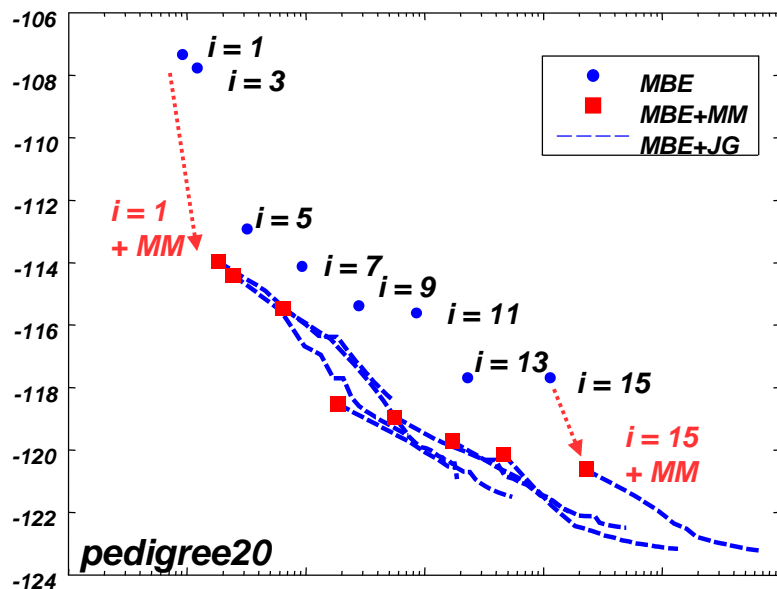
*$m_{11}, m_{12}$  - moment-matching messages*



*$MPE^*$  is an upper bound on MPE --U  
Generating a solution yields a lower bound--L*



# Anytime Approximation



- Can tighten the bound in various ways
  - Cost-shifting (improve consistency between cliques)
  - Increase  $i$ -bound (higher order consistency)

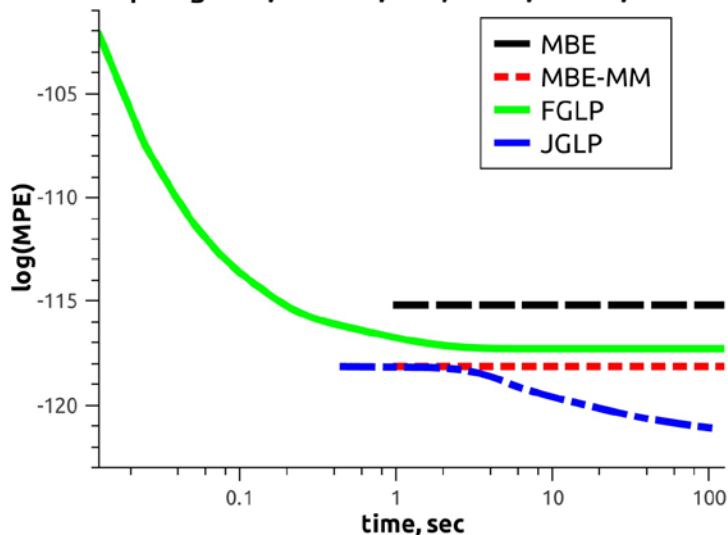


Simple moment-matching step improves bound significantly

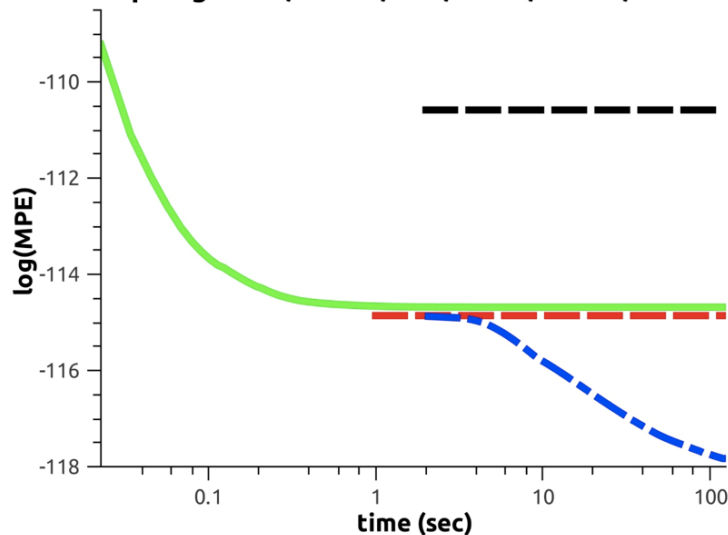


# Iterative tightening as bounding schemes

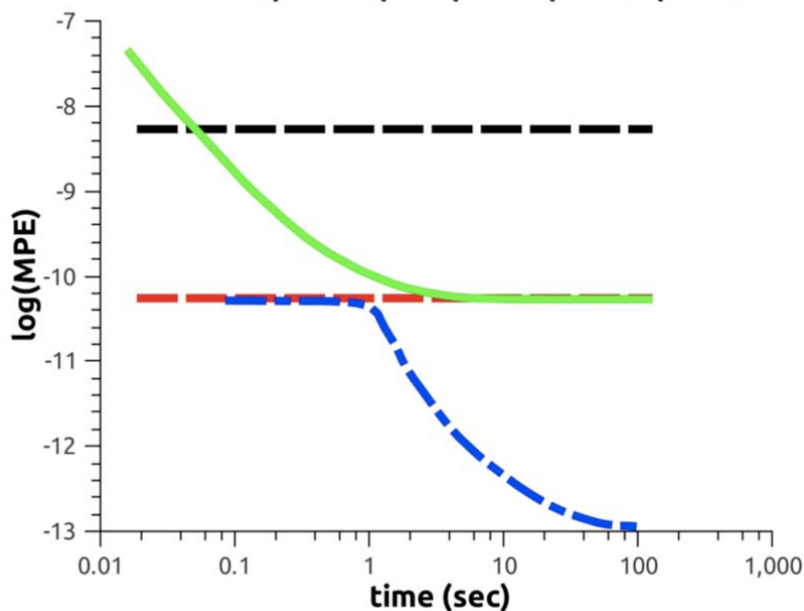
pedigree9, n=1119, k=5, w=25, h=123, z=10



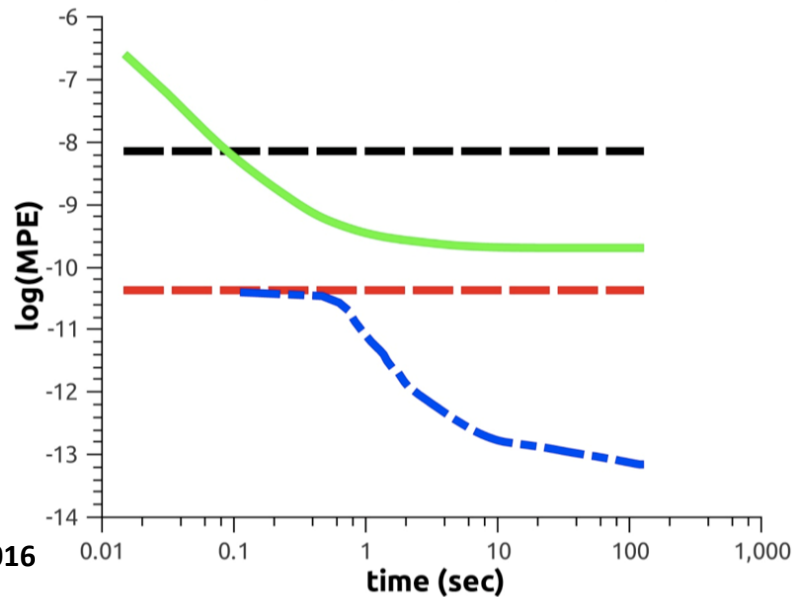
pedigree41, n=885, k=5, w=33, h=100, z=10



90-30-5, n=900, k=2, w=42, h=151, z=10



90-34-5, n=1156, k=2, w=48, h=186, z=10



*mm*

# Outline

- Graphical models, Queries, Algorithms
- Inference Algorithms: bucket-elimination
- Bounded Inference: a) mini-bucket, b) cost-shifting
- **Generating heuristics using mini-bucket elimination**
- AND/OR search spaces and AND/OR BnB
- Evaluation, Software
- Conclusions



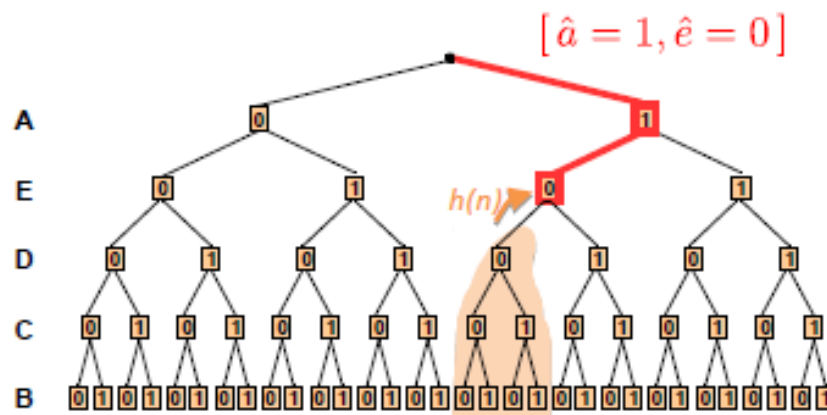
# Generating Heuristics for Graphical Models

Given a cost function:

$$f(a, \dots, e) = f(a) + f(a, b) + f(a, c) + f(a, d) + f(b, c) + f(b, d) + f(b, e) + f(c, e)$$

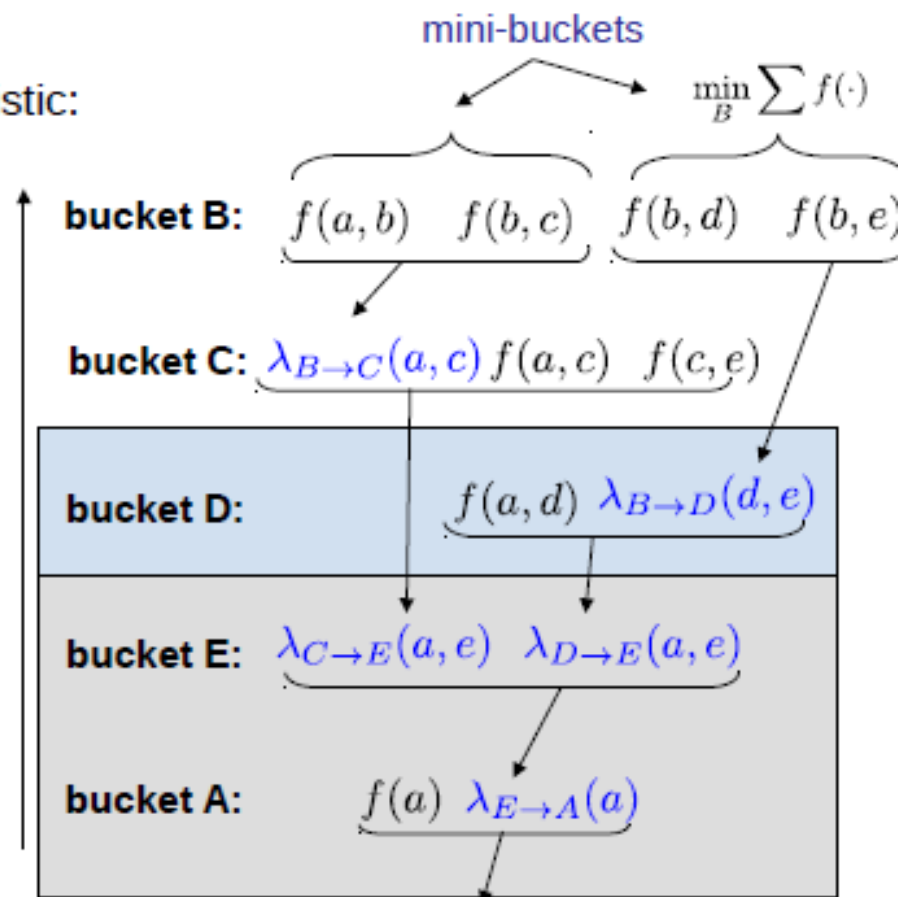
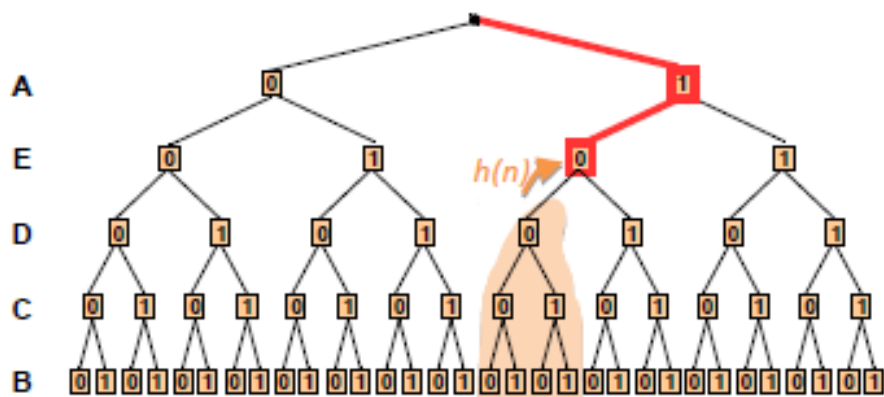
define an evaluation function over a partial assignment as the cost of its best extension:

$$\begin{aligned} f^*(\hat{a}, \hat{e}, D) &= \min_{b,c} F(\hat{a}, b, c, D, \hat{e}) \\ &= \underbrace{f(\hat{a})}_{g(\hat{a}, \hat{e}, D)} + \underbrace{\min_{b,c} f(\hat{a}, b) + f(\hat{a}, c) + \dots}_{h^*(\hat{a}, \hat{e}, D)} \\ &= g(\hat{a}, \hat{e}, D) + h^*(\hat{a}, \hat{e}, D) \end{aligned}$$



# Static Mini-Bucket Heuristics

Given a partial assignment,  $[\hat{a} = 1, \hat{e} = 0]$   
(weighted) mini-bucket gives an admissible heuristic:

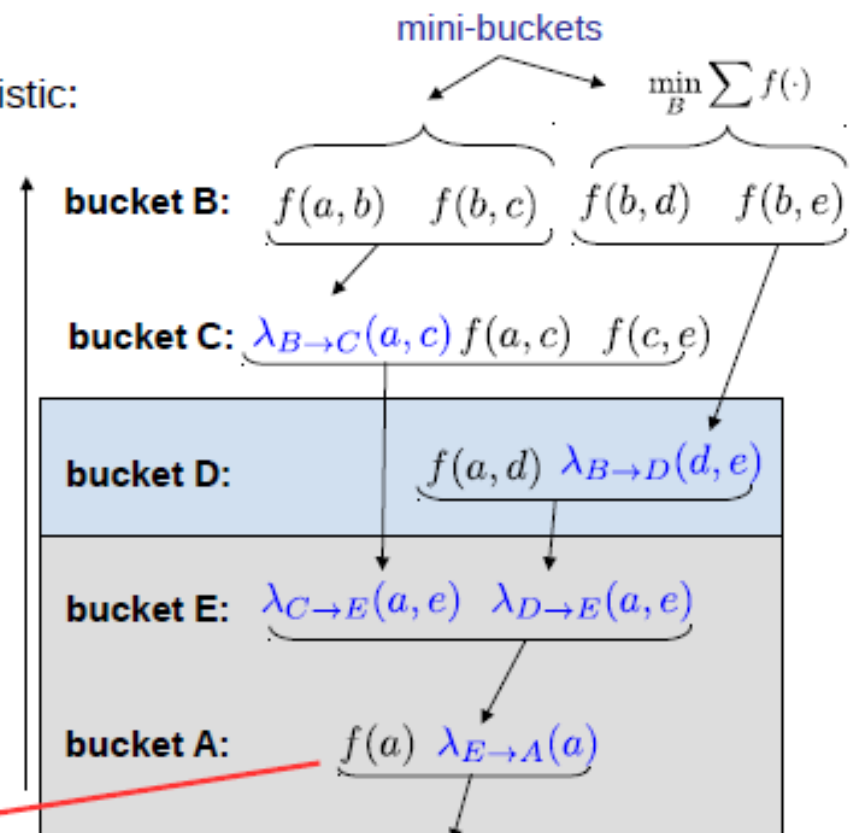
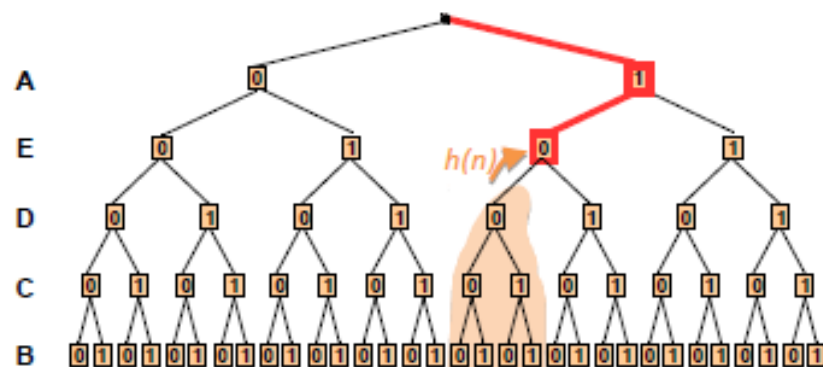


**L = lower bound**



# Static Mini-Bucket Heuristics

Given a partial assignment,  $[\hat{a} = 1, \hat{e} = 0]$   
(weighted) mini-bucket gives an admissible heuristic:



cost so far:

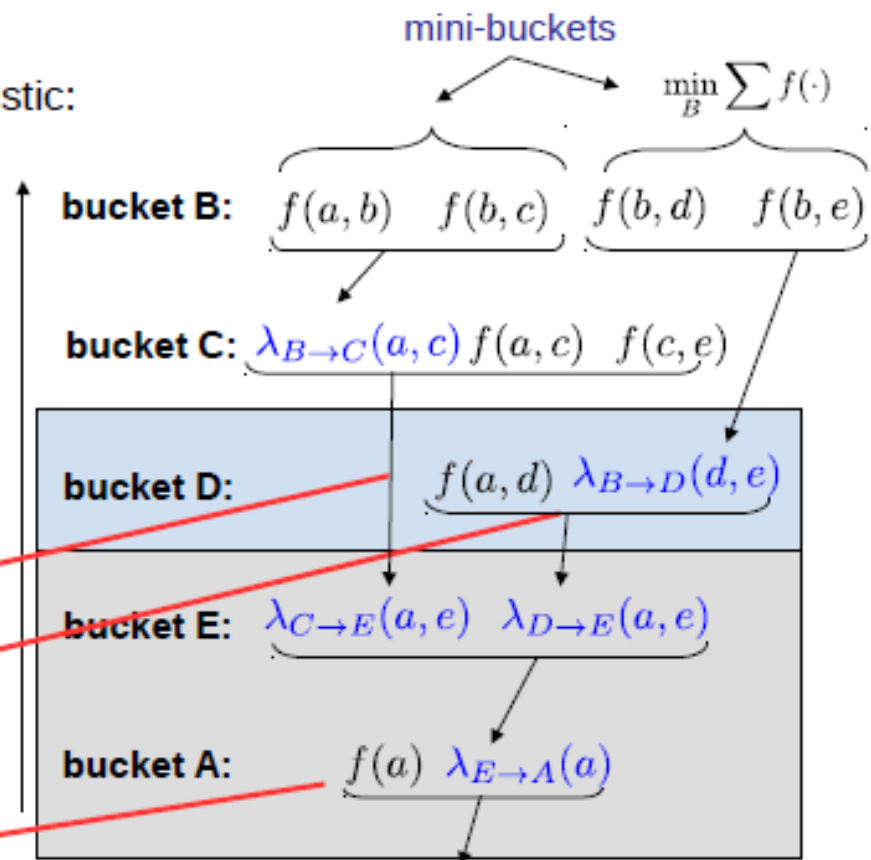
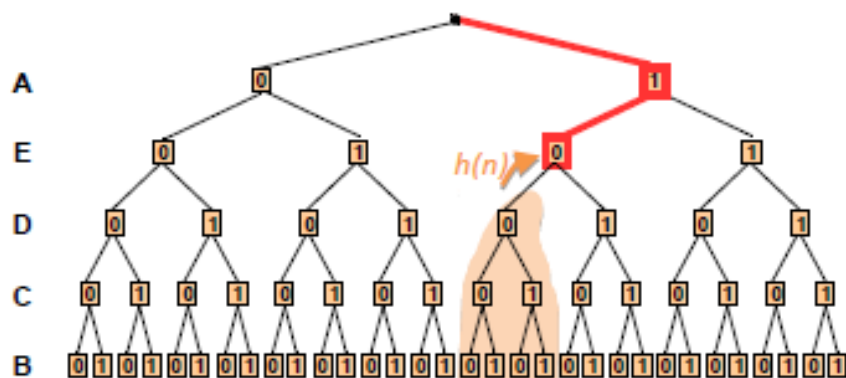
$$g(\hat{a}, \hat{e}) = f(A = \hat{a})$$

**L = lower bound**



# Static Mini-Bucket Heuristics

Given a partial assignment,  $[\hat{a} = 1, \hat{e} = 0]$   
(weighted) mini-bucket gives an admissible heuristic:



cost to go:

$$\tilde{h}(\hat{a}, \hat{e}, D) = \lambda_{C \rightarrow E}(\hat{a}, \hat{e}) + f(\hat{a}, D) + \lambda_{B \rightarrow D}(D, \hat{e})$$

(admissible:  $\tilde{h}(\hat{a}, \hat{e}, D) \leq h^*(\hat{a}, \hat{e}, D)$ )

cost so far:

$$g(\hat{a}, \hat{e}) = f(A = \hat{a})$$

**L = lower bound**



# Properties of the Heuristic

- MB heuristic is monotone, admissible
- Computed in linear time
- **IMPORTANT**
  - Heuristic strength can vary by MB(i) & message passing
  - Higher i-bound → more pre-processing
    - more accurate heuristic
    - less search
- Allows controlled trade-off between pre-processing and search



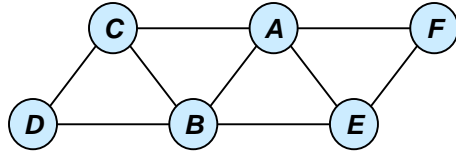
# Outline

- Graphical models, Queries , Algorithms
- Inference Algorithms
- Bounded Inference: mini-bucket, cost-shifting
- **AND/OR search spaces and AND/OR BnB**
- Evaluation, Software
- Conclusions



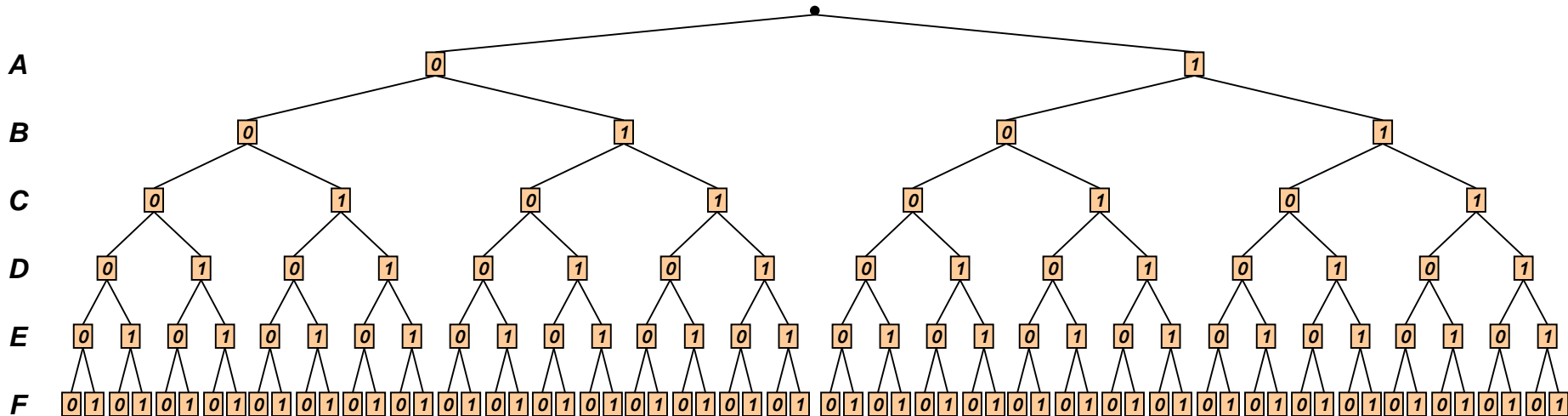


# Classic OR Search Space

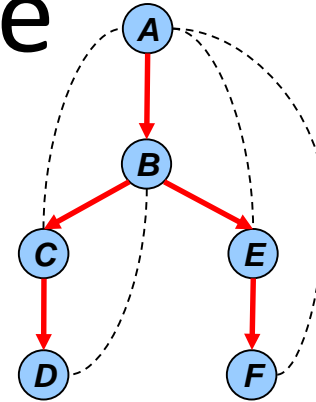
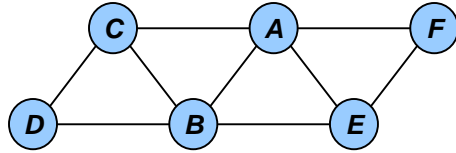


A	B	f <sub>1</sub>	A	C	f <sub>2</sub>	A	E	f <sub>3</sub>	A	F	f <sub>4</sub>	B	C	f <sub>5</sub>	B	D	f <sub>6</sub>	B	E	f <sub>7</sub>	C	D	f <sub>8</sub>	E	F	f <sub>9</sub>
0	0	2	0	0	3	0	0	0	0	0	2	0	0	0	0	0	4	0	0	3	0	0	1	0	0	1
0	1	0	0	1	0	0	1	3	0	1	0	0	1	1	0	1	2	0	1	2	0	1	4	0	1	0
1	0	1	1	0	0	1	0	2	1	0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

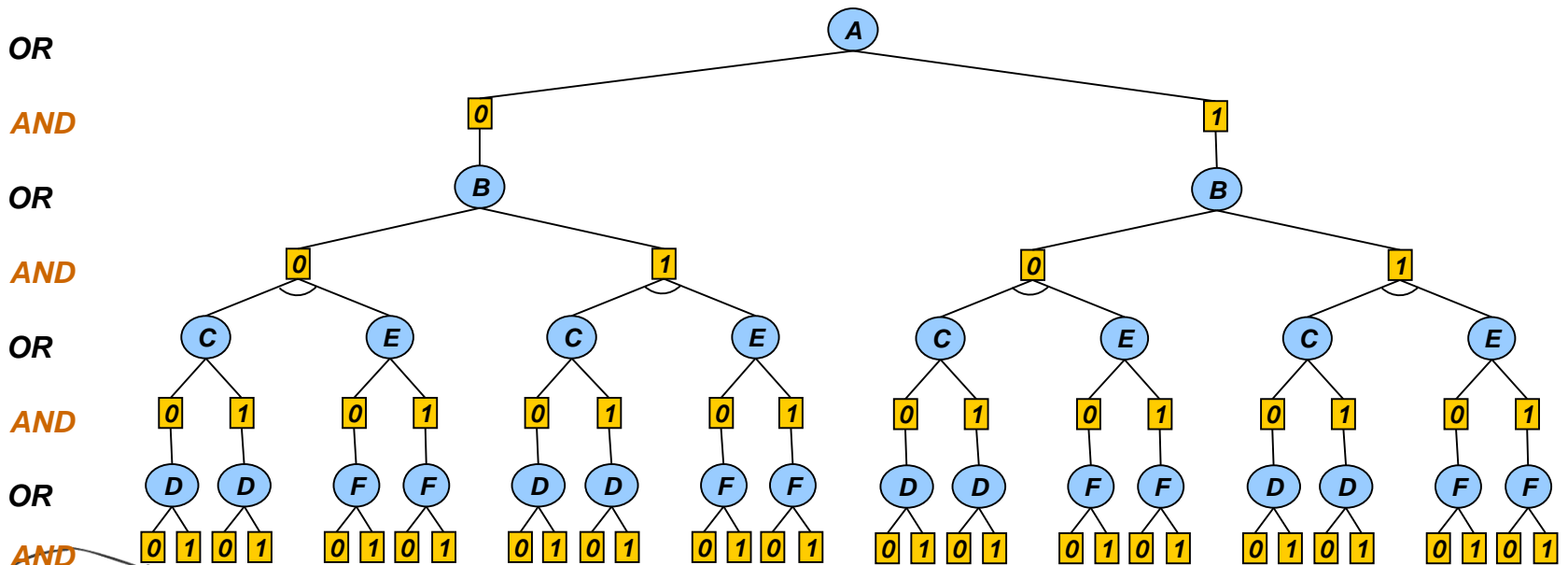
**Objective function:**  $F^* = \min_x \sum_{i=1}^9 f_i(X)$



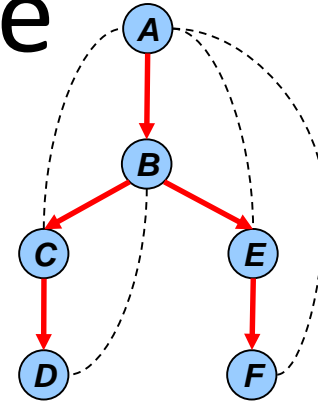
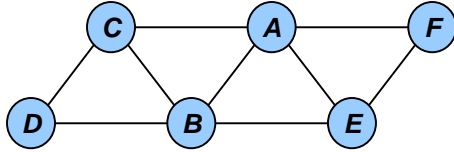
# The AND/OR Search Tree



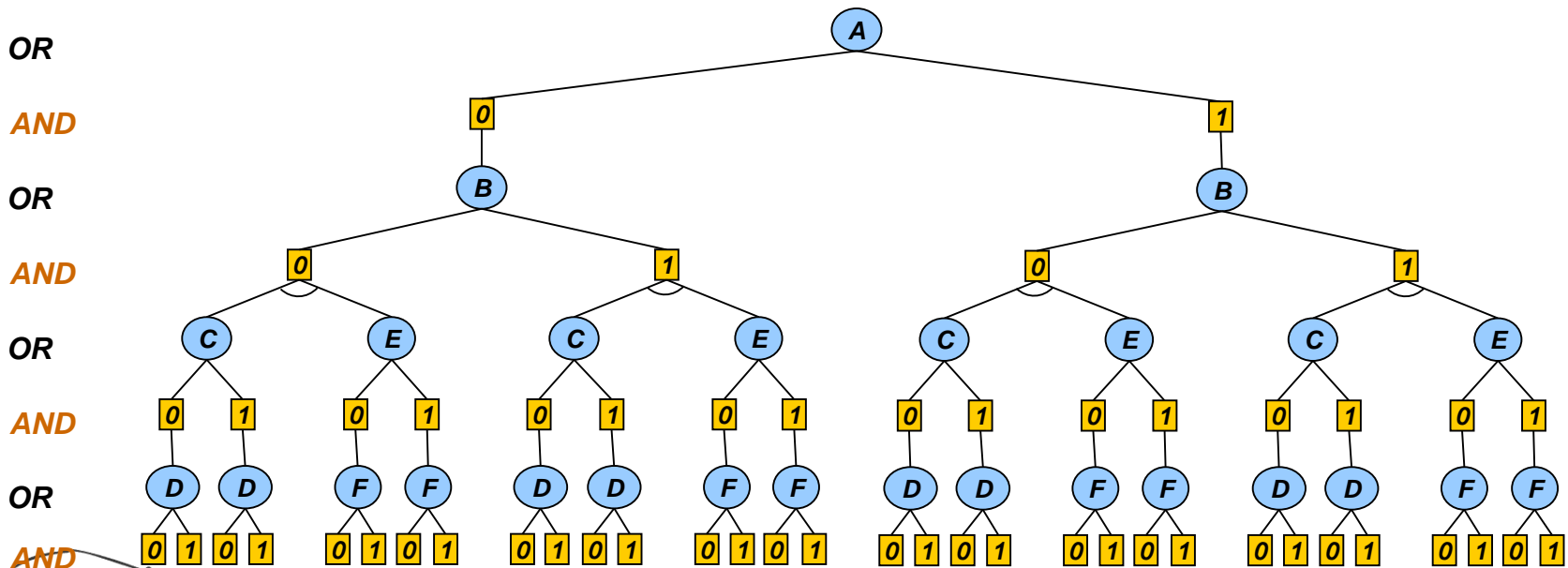
*Pseudo tree (Freuder & Quinn85)*



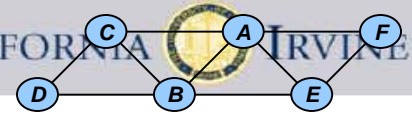
# The AND/OR Search Tree



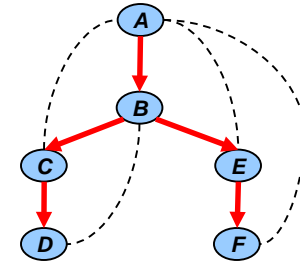
*Pseudo tree*



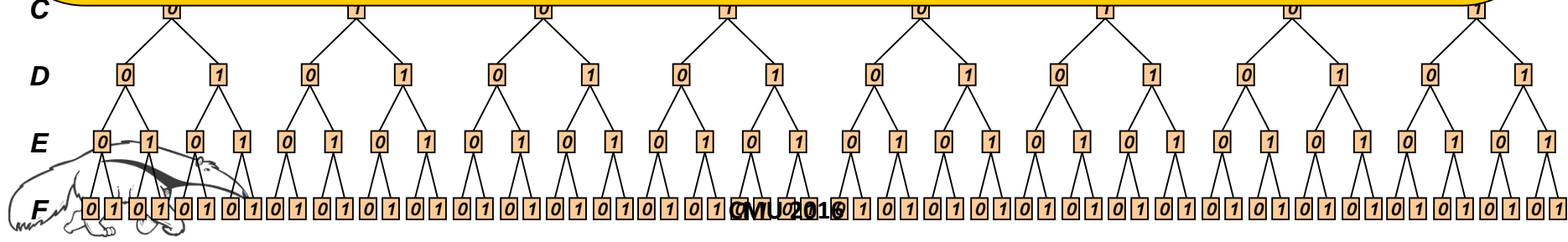
A solution subtree is  $(A=0, B=1, C=0, D=0, E=1, F=1)$



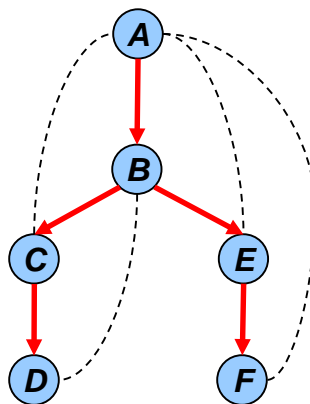
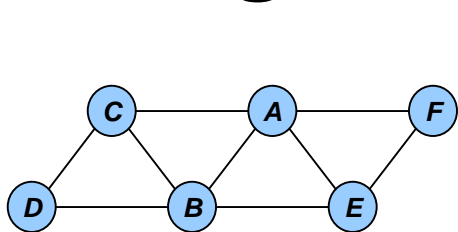
# AND/OR vs. OR Spaces



**Time  $O(nk^h)$**   
**Space  $O(n)$**   
**height is bounded by  $(\log n) w^*$**

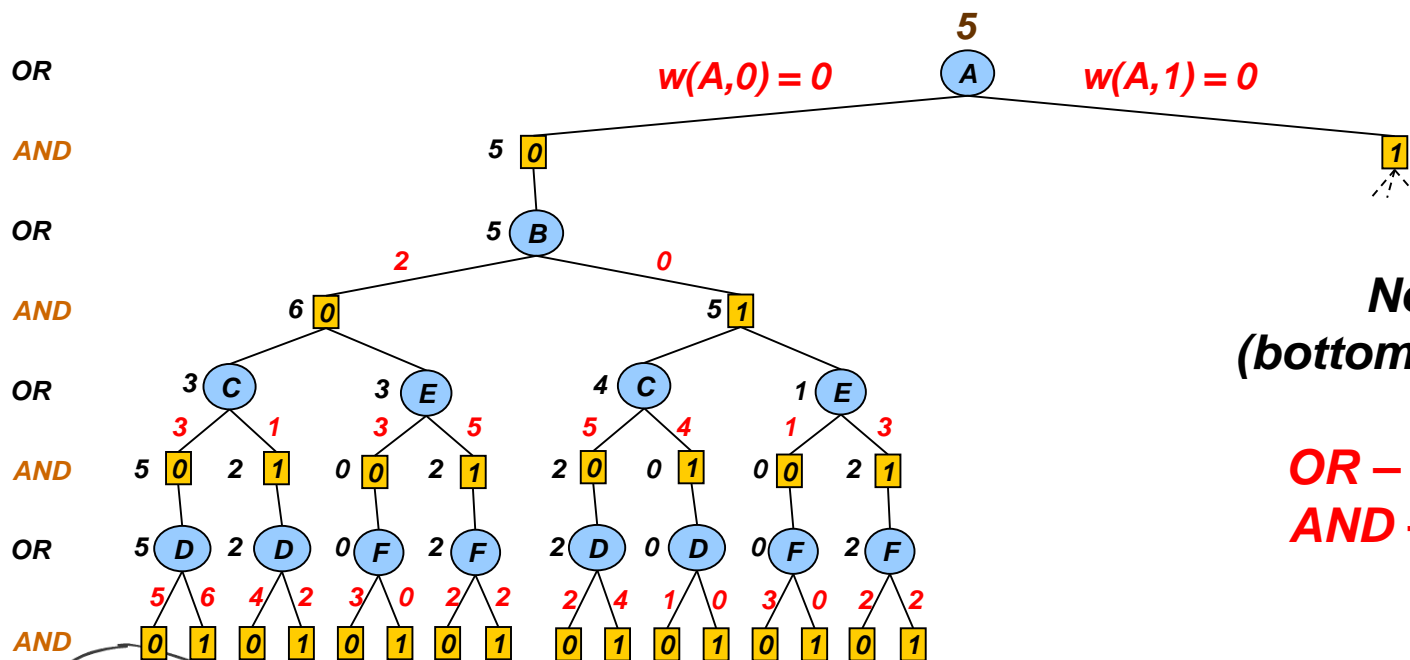


# Weighted AND/OR Search Tree



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	1
0	1	0	0	1	0	0	1	3	0	1	0	0	1	1	0	1	2	0	1	2	0	1	4	0	1	0
1	0	1	1	0	0	1	0	2	1	0	0	1	0	2	1	0	1	1	0	1	1	0	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	2

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

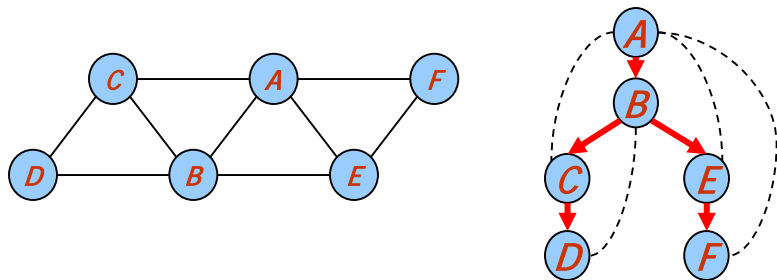


**Node Value**  
*(bottom-up evaluation)*

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

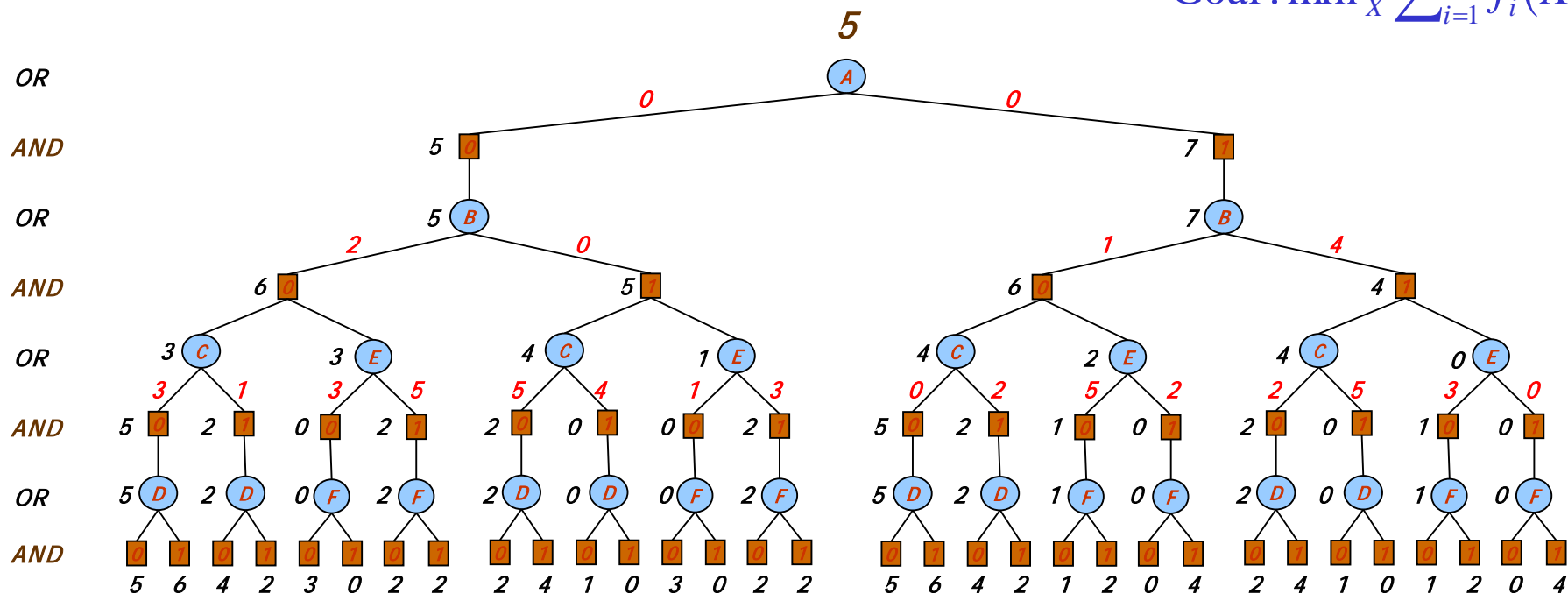


# Weighted AND/OR Search Tree



AB	$f_1$	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	$f_9$
00	2	00	3	00	0	00	2	00	0	00	4	00	3	00	1	00	1
01	0	01	0	01	3	01	0	01	1	01	2	01	2	01	4	01	0
10	1	10	0	10	2	10	0	10	2	10	1	10	1	10	0	10	0
11	4	11	1	11	0	11	2	11	4	11	0	11	0	11	0	11	2

Goal :  $\min_x \sum_{i=1}^9 f_i(X)$



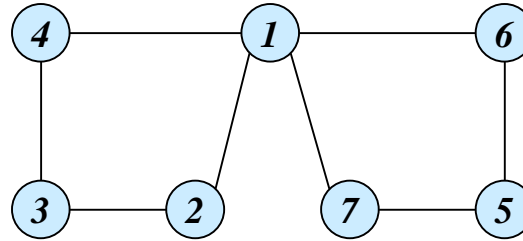
**AND node = Combination operator (summation)**

**OR node = Marginalization operator (minimization)**



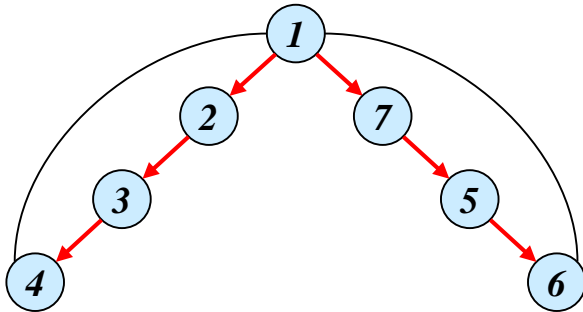
# Pseudo-Trees

(Freuder 85, Bayardo 95, Bodlaender and Gilbert, 91)

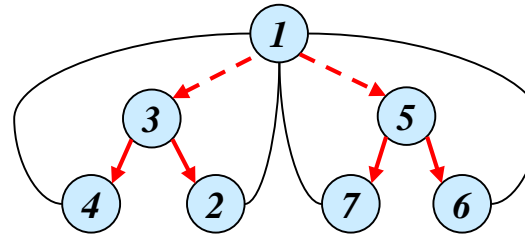


(a) Graph

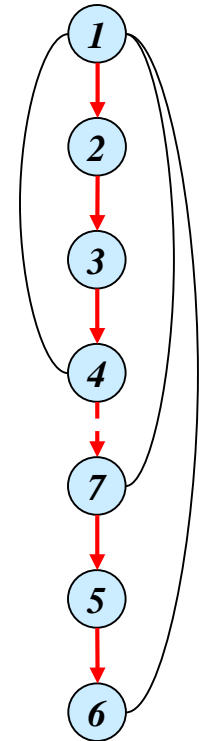
$$m \leq w * \log n$$



(b) DFS tree  
depth=3



(c) pseudo-tree  
depth=2

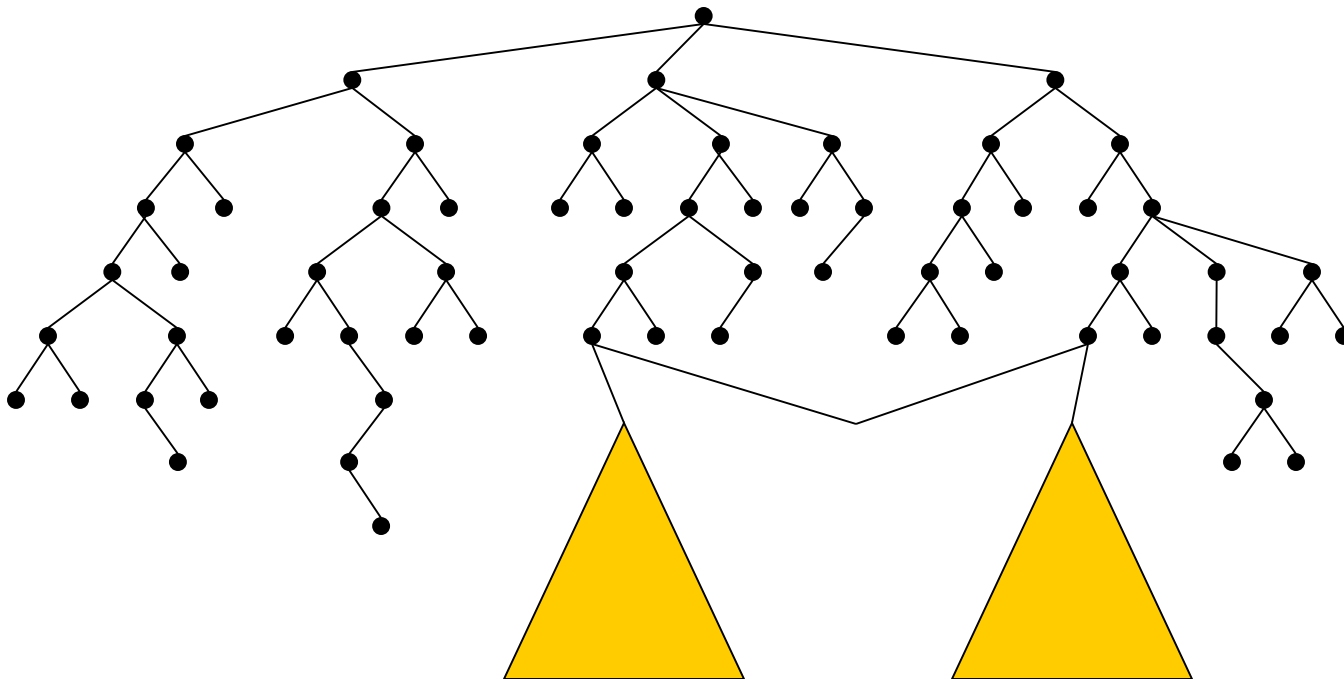


(d) Chain  
depth=6



# From Search Trees to Search Graphs

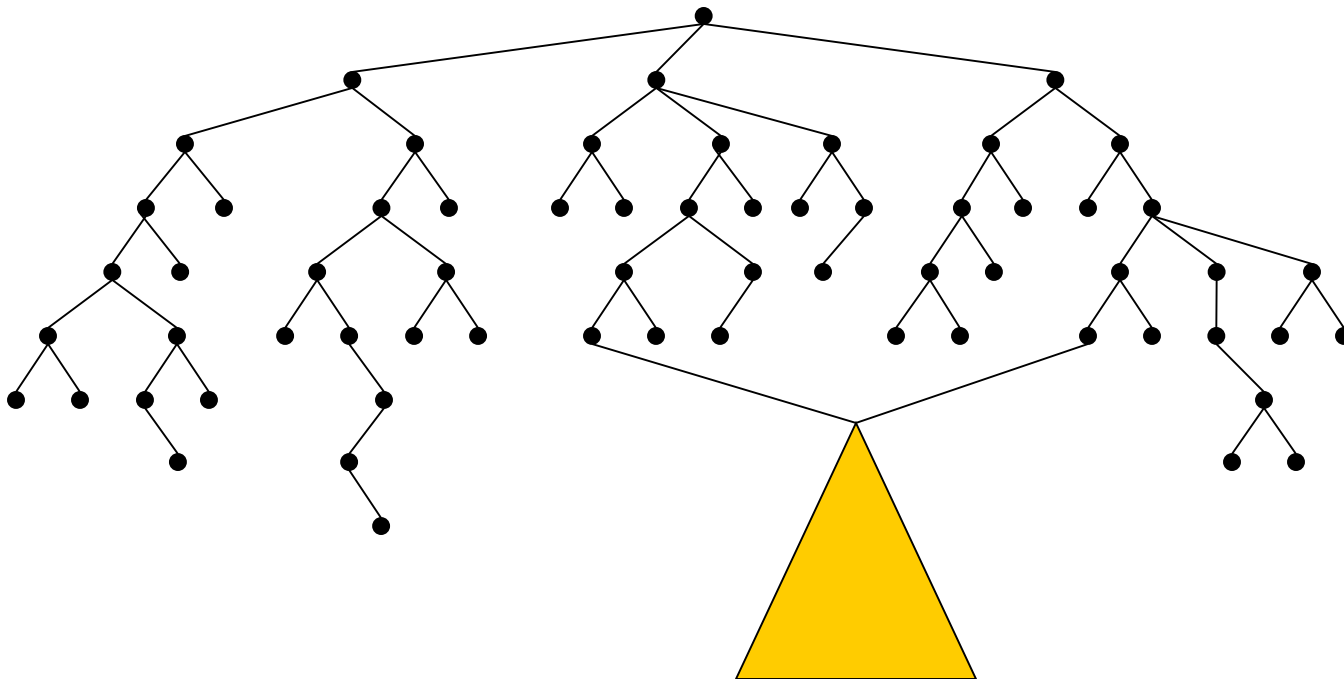
- Any two nodes that root **identical** sub-trees or sub-graphs can be **merged**



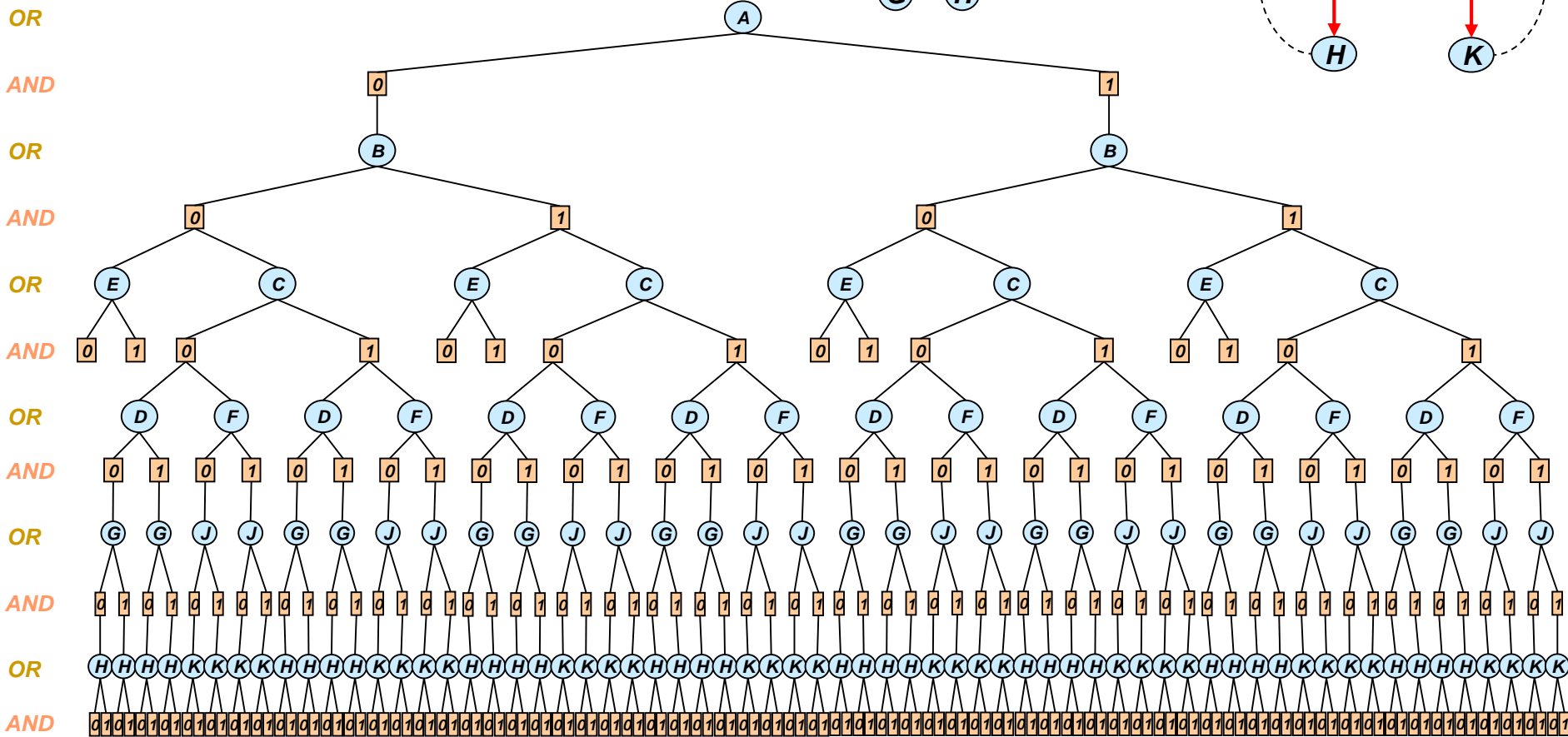
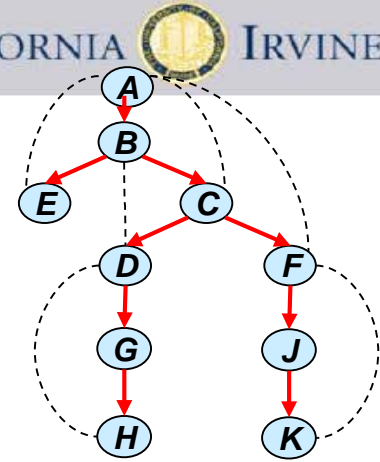
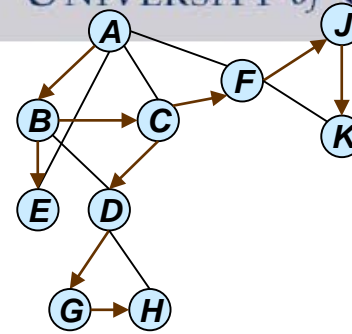


# From Search Trees to Search Graphs

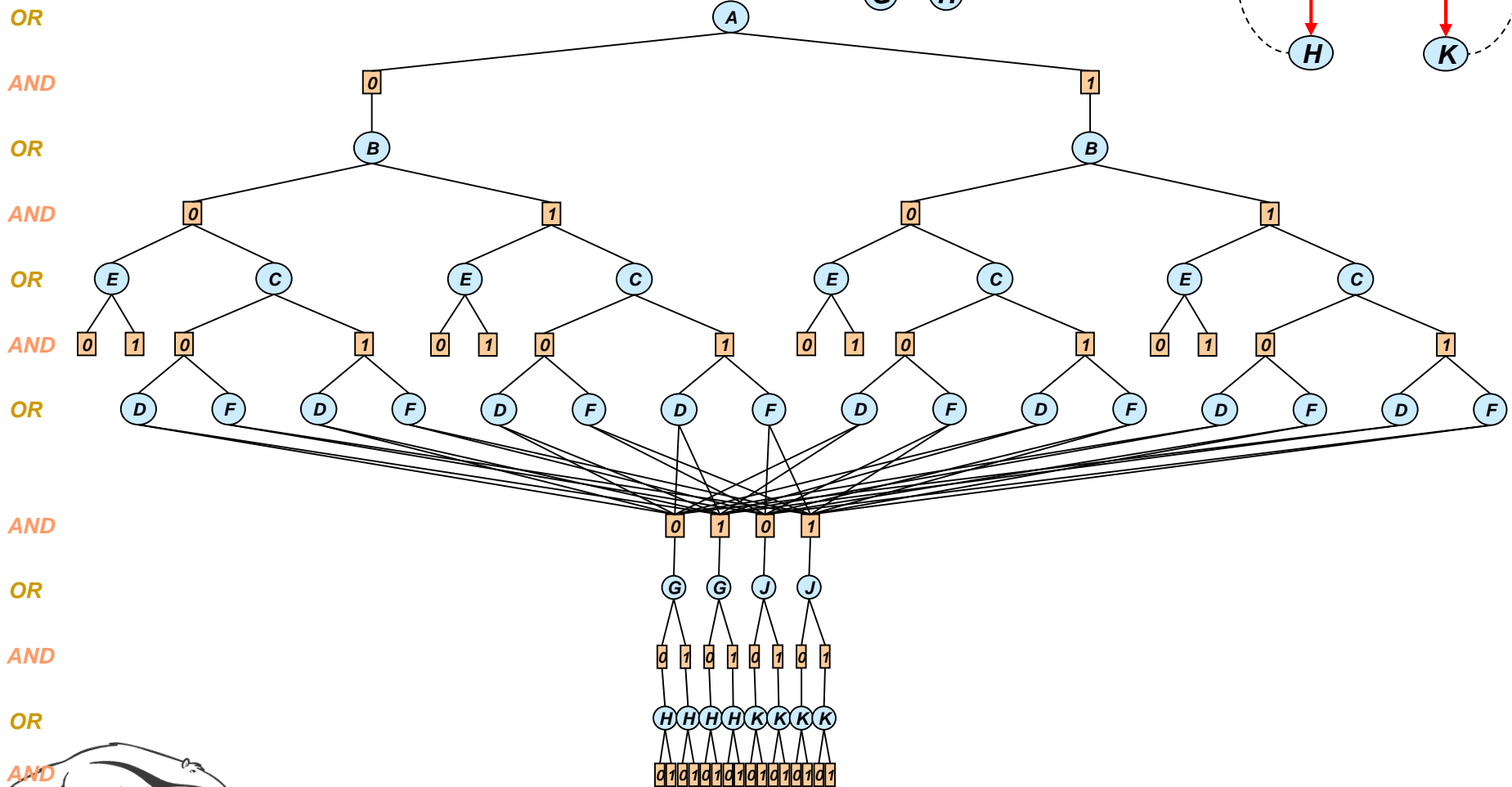
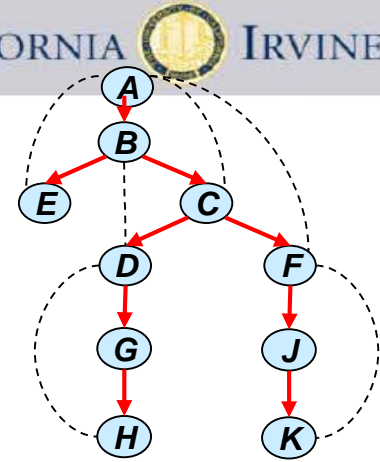
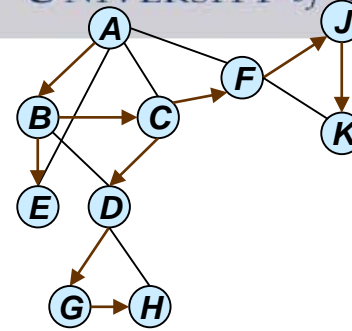
- Any two nodes that root **identical** sub-trees or sub-graphs can be **merged**



# From AND/OR Tree



# An AND/OR Graph



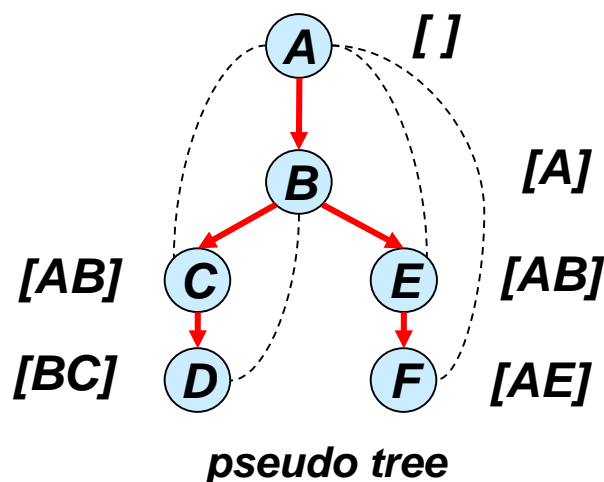
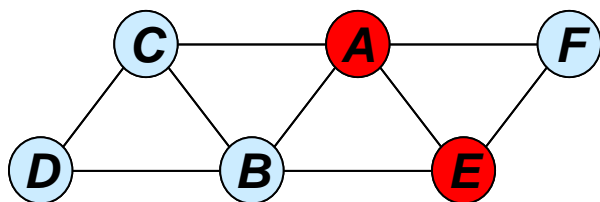
CMU 2016



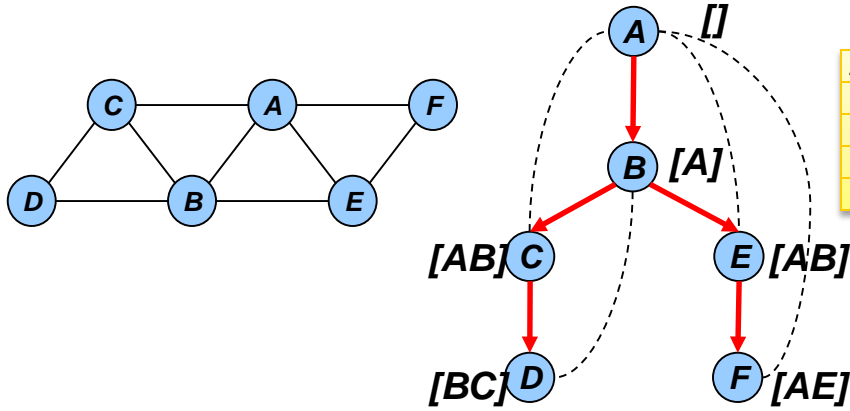
# Merging Based on Context

- One way of recognizing nodes that can be merged (based on graph structure)

**context(X)** = ancestors of X in the pseudo tree that are connected to X, or to descendants of X

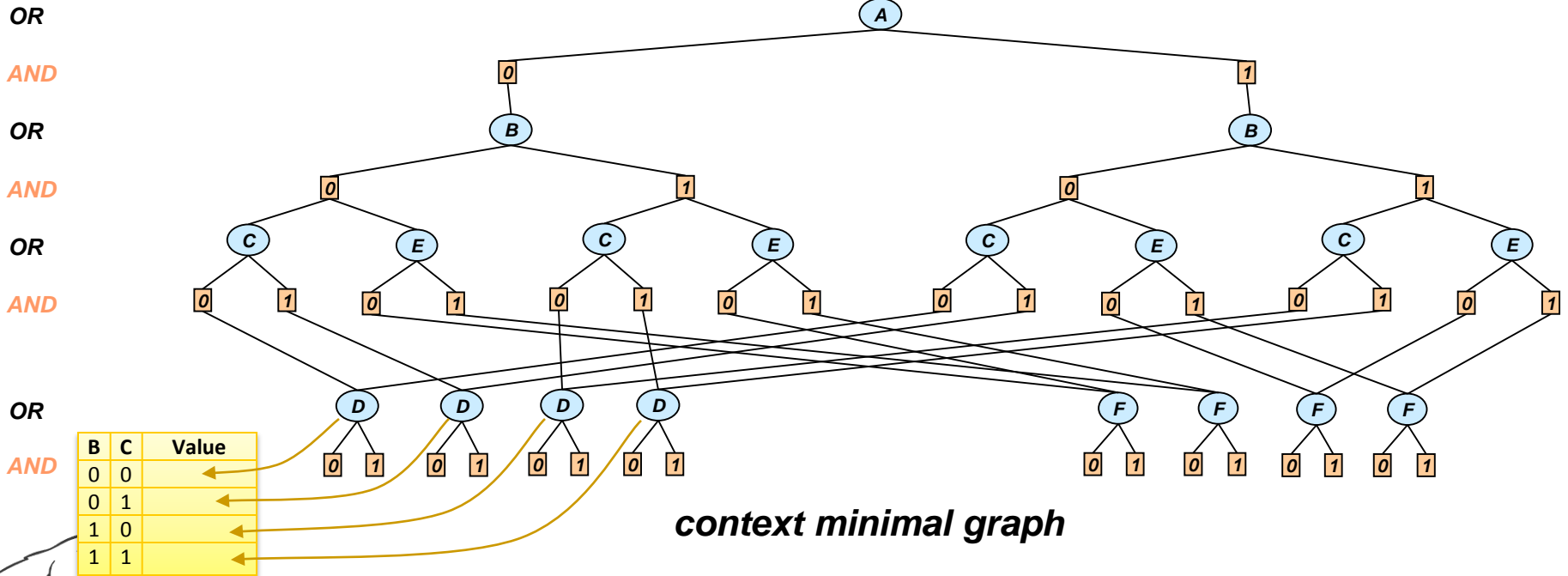


# AND/OR Search Graph



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	2	0	1	2	0	1	4	0	1	0
1	0	1	1	0	0	1	0	2	1	0	0	1	0	2	1	0	1	1	0	1	1	0	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	2

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



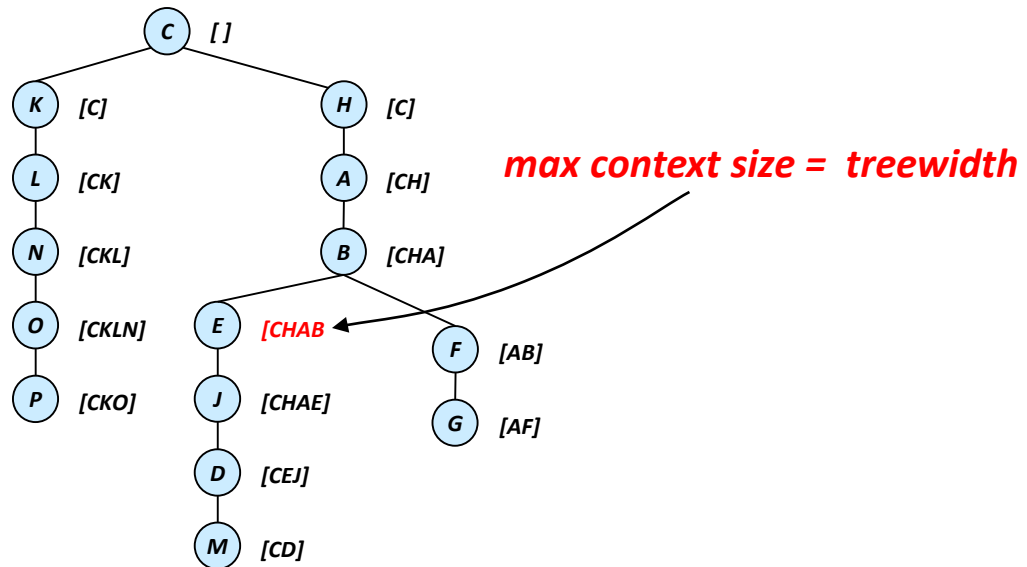
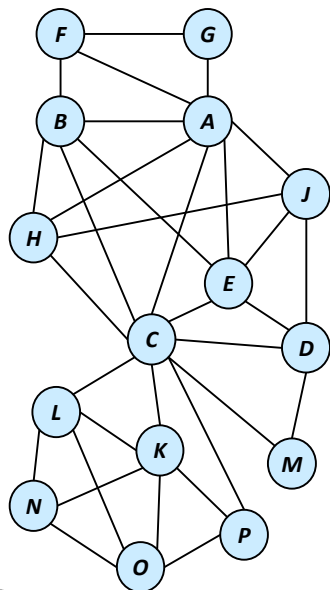
context minimal graph

B	C	Value
0	0	←
0	1	←
1	0	←
1	1	←

Cache table for D

# How Big Is The Context?

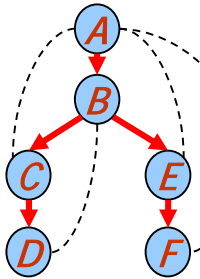
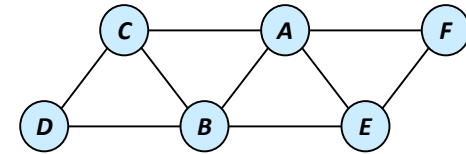
**Theorem:** The maximum **context** size for a pseudo tree is equal to the **treewidth** of the graph along the pseudo tree.



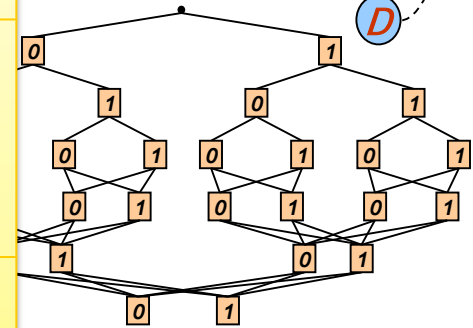
**(CKHABEJLNODP MFG)**



# All Four Search Spaces



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



next minimal OR search graph

28 nodes

AND  
OR  
AND  
OR  
AND  
OR  
AND

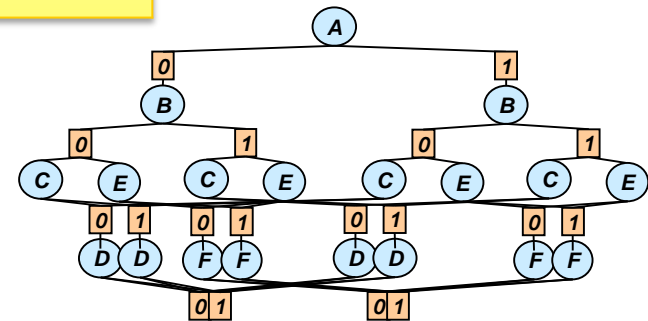


Computes any query:

- Constraint satisfaction
- Optimization
- Weighted counting

34 AND nodes

OR  
AND  
OR  
AND  
OR  
AND  
OR  
AND



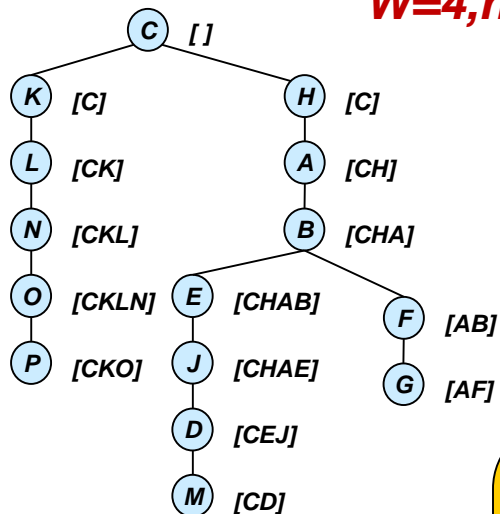
Context minimal AND/OR search graph

18 AND nodes



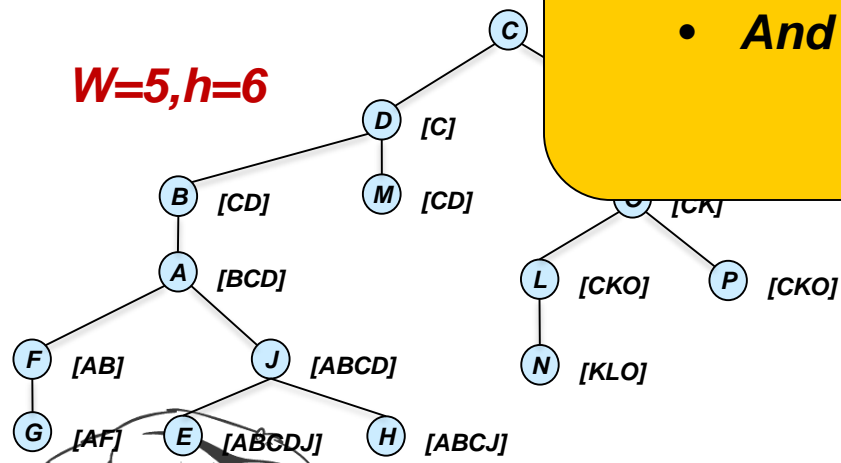
# The impact of the pseudo-tree

$W=4, h=8$



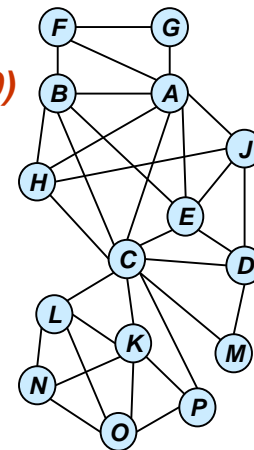
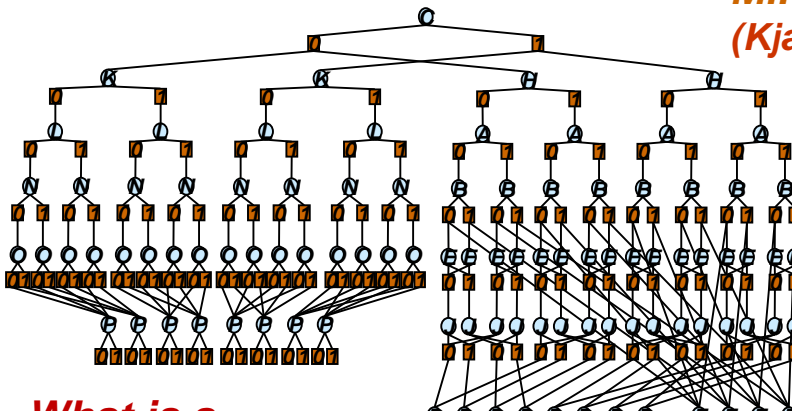
(CKHABEJLNODPM)

$W=5, h=6$



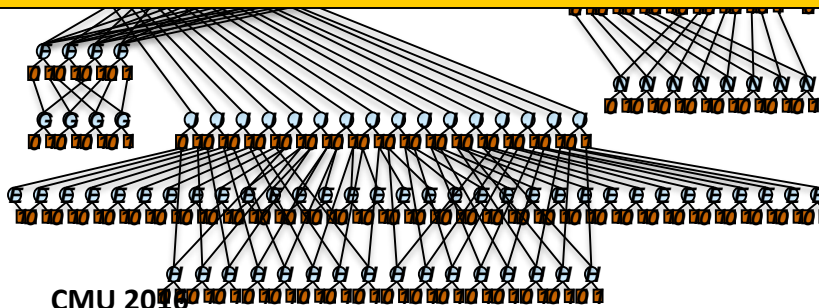
(CDKBAOMLNPJHEFG)

Min-Fill  
(Kjaerulff90)



**Optimization**

- Choose pseudo-tree with a minimal search graph
- But determinism is unpredictable
- And pruning by BnB is even more unpredictable



CMU 2016



# Outline

- Graphical models, Queries, Algorithms
- Inference Algorithms: bucket-elimination
- Bounded Inference: a) mini-bucket, b) cost-shifting
- AND/OR search spaces and **AND/OR Branch & Bound**
- Evaluation, Software
- Summary and future work



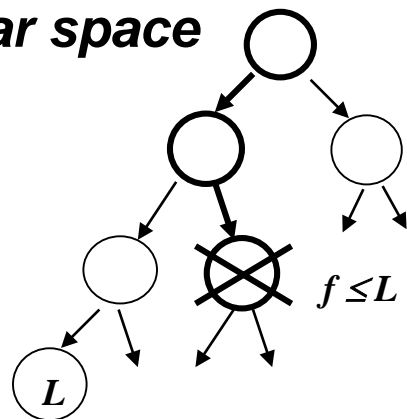
# Basic Heuristic Search Schemes

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

## 1. Branch-and-Bound

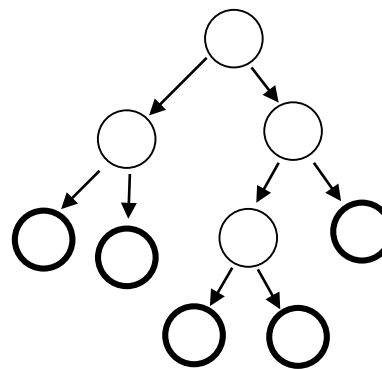
**Use heuristic function  $f(x^p)$  to prune the depth-first search tree**

**Linear space**



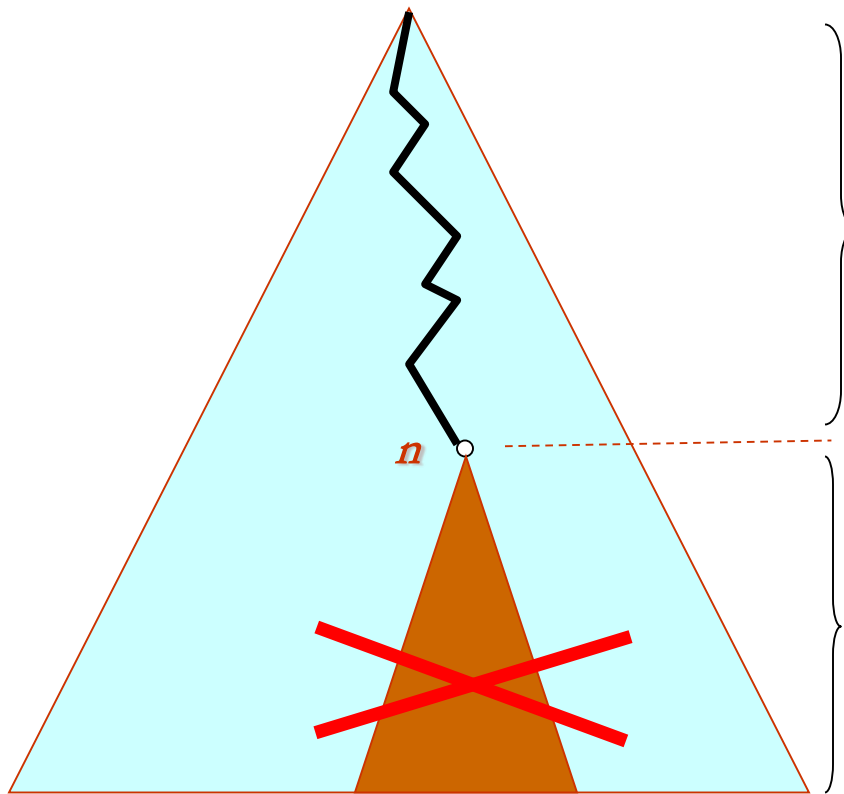
## 2. Best-First Search

**Always expand the node with the highest heuristic value  $f(x^p)$  needs lots of memory**



# Classic Branch-and-Bound

*Each node is a COP subproblem  
(defined by current conditioning)*



$g(n)$

$$f(n) = g(n) + h(n)$$

$f(n) = \text{lower bound}$

**Prune if  $f(n) \geq UB$**

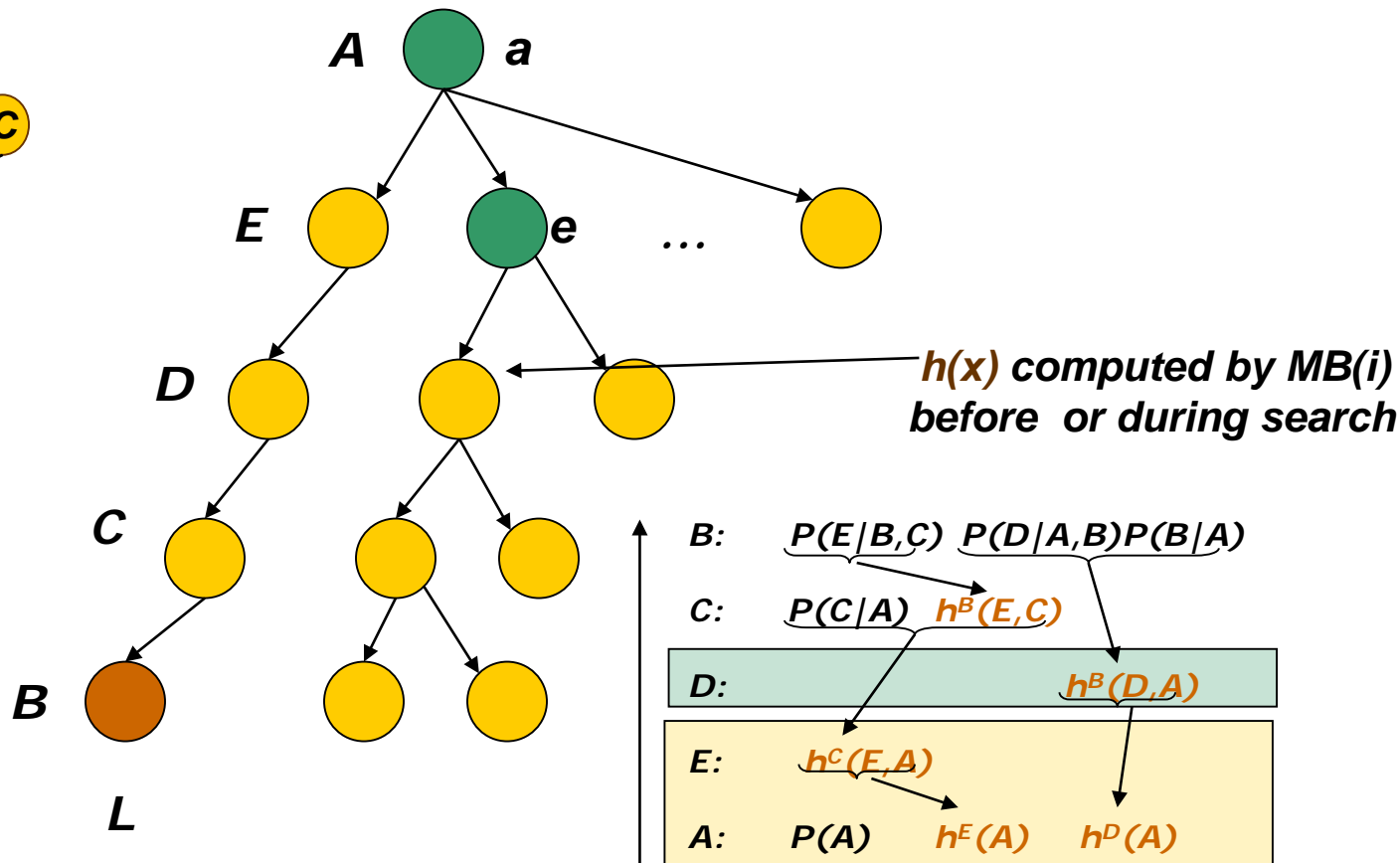
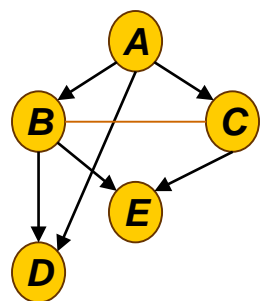
$h(n)$  - under-estimates  
Optimal cost below  $n$



**(UB) Upper Bound = best solution so far**

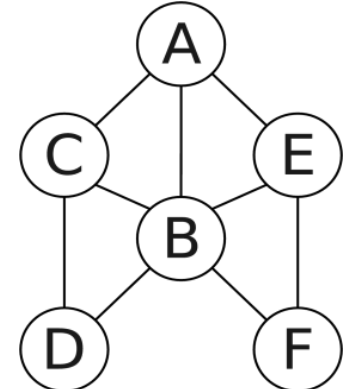
# Mini-bucket Heuristics for BB search

( Kask and dechterAIJ, 2001, Kask, Dechter and Marinescu 2004, 2005, 2009, Otten 2012)



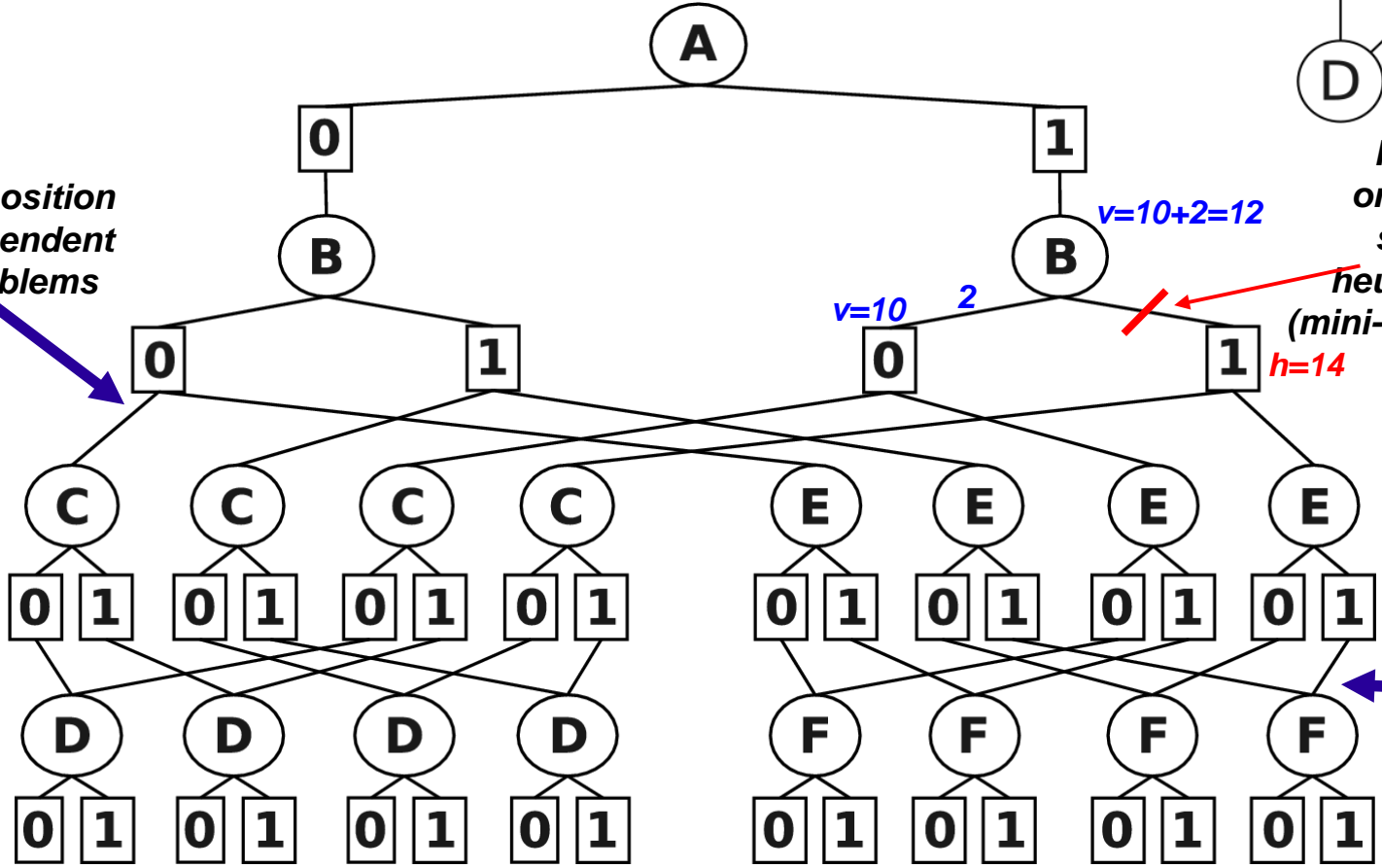
$$f(a,e,D) = P(a) \cdot h^B(D,a) \cdot h^C(e,a)$$

# AND/OR Branch-and-Bound



Prune based on current best solution and heuristic estimate (mini-bucket heuristic).

Decomposition of independent subproblems



Cache table for F (independent of A)

B	E	cost
0	0	10
0	1	6
1	0	...
1	1	...



# MAP: Anytime, Branch & Bound

- Best-First, Recursive Best-First
- Anytime:
  - Breadth-Rotate AND/OR BnB (2011)
  - Weighted heuristic AND/OR search (2014)
- Finding m-best solutions
- Marginal map



# Empirical Evaluation (exact)

***Grid and Pedigree benchmarks; Time limit 1 hour.***



# Outline

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- AND/OR search spaces and AND/OR BnB
- **Evaluation, Software**
- Conclusion





# PASCAL 2012 Inference Challenge

## DAOOPT: Improving AND/OR Branch-and-Bound for Graphical Models

(also won 2<sup>nd</sup> place uai 2014 as is)

*Lars Otten, Alexander Ihler,  
Kalev Kask, Rina Dechter*

*Dept. of Computer Science  
University of California, Irvine*



# Our Solvers are being used:

- Superlink online, software for linkage analysis (Geiger et. Al)
- Figaro, probabilistic language (Avi Pfeffer)



# Software

- **aolib**
  - <http://graphmod.ics.uci.edu/group/Software>  
(standalone AOBB, AOBF solvers)
- **daoopt**
  - <https://github.com/lotten/daoopt>  
(distributed and standalone AOBB solver)



# UAI Probabilistic Inference Competitions

- **2006**  (*aolib*)
- **2008**  (*aolib*)
- **2011**  (*daoopt*)
- **2014**  (*daoopt*)

**MPE/MAP**

-  (*daoopt*)  (*merlin*)

**MMAF**



# Conclusion

- Combining two “universal” lower-bounds scheme (mpe/map)
  - The mini-bucket scheme
  - cost-shifting or re-parameterization, schemes
- Exploiting bounds as heuristics in AND/OR search
- Yields BRAOBB that wins first place Pascal competition 2011, over many benchmarks
- **Future work: Dynamic heuristics and search spaces**



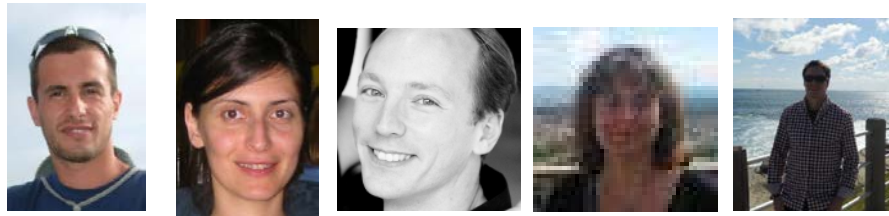
Reasoning with Probabilistic  
and Deterministic  
Graphical Models  
*Exact Algorithms*

Rina Dechter

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