Chapter 13

Constraint Optimization
And counting, and enumeration
275 class

Outline

Introduction

- Optimization tasks for graphical models
- Solving optimization problems with inference and search

Inference

- Bucket elimination, dynamic programming
- Mini-bucket elimination

Search

- Branch and bound and best-first
- Lower-bounding heuristics
- AND/OR search spaces

Hybrids of search and inference

- Cutset decomposition
- Super-bucket scheme

Constraint Satisfaction

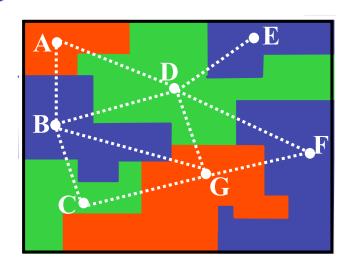
Example: map coloring

Variables - countries (A,B,C,etc.)

Values - colors (e.g., red, green, yellow)

Constraints: $(A \neq B)$, $A \neq D$, $D \neq E$, etc.

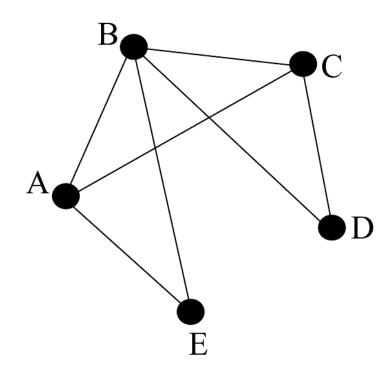
A	В
red	green
red	yellow
green	red
green	yellow
yellow	green
yellow	red



Task: consistency? Find a solution, all solutions, counting

Propositional Satisfiability

 $\varphi = \{(\neg C), (A \lor B \lor C), (\neg A \lor B \lor E), (\neg B \lor C \lor D)\}.$



Constraint Optimization Problems for Graphical Models

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

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

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

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

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

Α	В	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

Global Cost Function

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

Constraint Optimization Problems for Graphical Models

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 - variables

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

A	В	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

$$F(a,b,c,d,f,g) = f1(a,b,d) + f2(d,f,g) + f3(b,c,f)$$

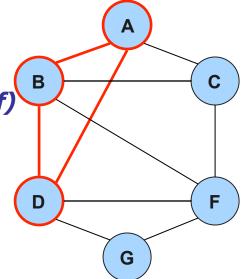
f1(A,B,D)

f2(D,F,G)

f3(B,C,F)

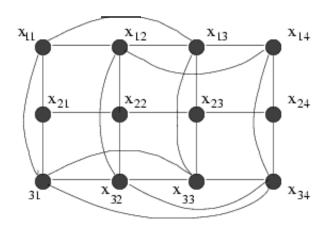
Global Cost Function

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



Constrained Optimization

Example: power plant scheduling



Unit #	Min Up Time	Min Down Time
1	3	2
2	2	1
3	4	1

Variables = $\{X_1, ..., X_n\}$, domain = $\{ON, OFF\}$.

Constraints: $X_1 \vee X_2$, $\neg X_3 \vee X_4$, min - up and min - down time,

power demand: $\sum_{i=1}^{\infty} Power(X_i) \ge Demand$

Objective: minimize TotalFuelCost $(X_1,...,X_N)$

Graphical Models

A graphical model (**X**,**D**,**F**):

•
$$\mathbf{X} = \{X_1, ..., X_n\}$$
 variables

•
$$D = \{D_1, ... D_n\}$$
 domains

•
$$\mathbf{F} = \{f_1, ..., f_m\}$$
 functions

Operators:

- combination
- elimination (projection)

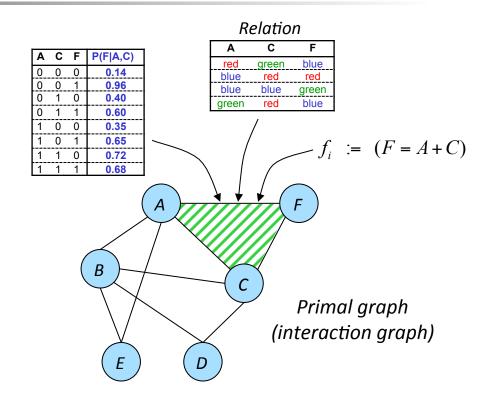
Tasks:

Belief updating: $\Sigma_{X-y} \prod_j P_i$

• **MPE**: $\max_{X} \prod_{i} P_{i}$

• CSP: $\prod_X \times_i C_i$

• Max-CSP: $min_{\chi} \Sigma_i f_i$



All these tasks are NP-hard

- exploit problem structure
- identify special cases
- approximate



Combination of Cost Functions

A	В	f(A,B)
b	b	6
b	g	0
g	b	0
g	g	6

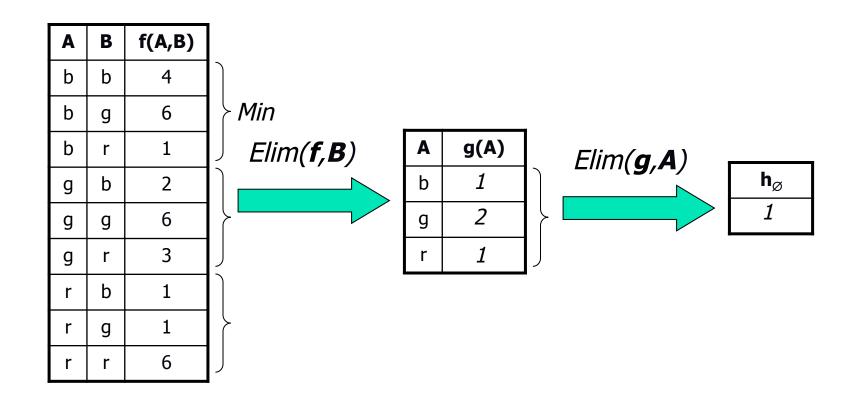


Α	В	С	f(A,B,C)
b	b	b	12
b	b	g	6
b	g	b	0
b	g	g	6
g	b	b	6
g	b	g	0
g	g	b	6
g	g	g	12

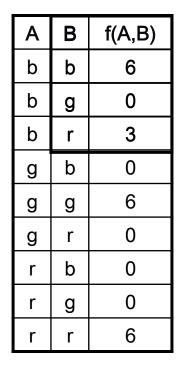
В	С	f(B,C)
b	b	6
b	g	0
g	b	0
g	g	6

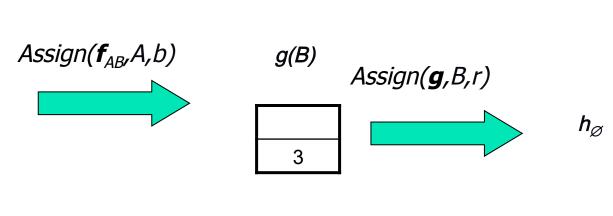
$$= 0 + 6$$

Elimination in a Cost Function



Conditioning a Cost Function





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- Solving by inference and search

Inference

- Bucket elimination, dynamic programming, treeclustering, bucket-elimination
- Mini-bucket elimination, belief propagation

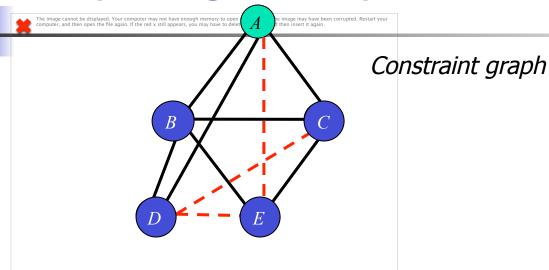
Search

- Branch and bound and best-first
- Lower-bounding heuristics
- AND/OR search spaces

Hybrids of search and inference

- Cutset decomposition
- Super-bucket scheme

Computing the Optimal Cost Solution



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

$$Combination$$

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



$$h^{B}(a,d,c,e)$$

Finding

$$OPT = \min_{X_1, \dots, X_n} \sum_{j=1}^r f_j(X)$$

Algorithm **elim-opt** (Dechter, 1996) Non-serial Dynamic Programming (Bertele and Briochi, 1973)

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

$$\min_{b} \sum_{c} \leftarrow Elimination \ operator$$

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

bucket C: $f(c,a) f(c,e) h^B (a,d,c,e)$

bucket D: $f(a,d) h^C (a,d,e)$

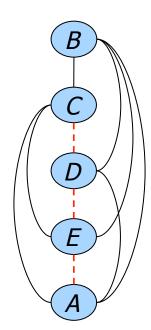
bucket E: $e=0 h^D (a,e)$

bucket A: $h^E (a)$

bucket C:
$$f(c,a) f(c,e)$$
 $h^B(a,d,c,e)$

bucket D:
$$f(a,d)$$
 h^c (a,d,e)

bucket E:
$$e=0$$
 $h^{D}(a,e)$



Generating the Optimal Assignment

5.
$$b' = arg \min_{b} f(a',b) + f(b,c') + f(b,d') + f(b,e')$$

4.
$$c' = arg \min_{c} f(c,a') + f(c,e') + h^{B}(a',d',c,e')$$

3.
$$d' = arg \min_{d} f(a',d) + h^{C}(a',d,e')$$

1.
$$a' = arg \min_{a} h^{E}(a)$$

C:
$$f(c,a) f(c,e)$$
 $h^B(a,d,c,e)$

$$D: f(a,d)$$
 $h^c(a,d,e)$

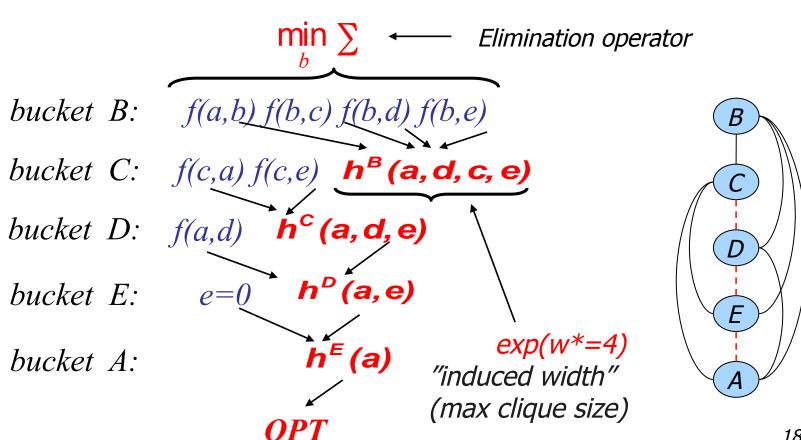
$$E: e=0$$
 $h^{D}(a,e)$

$$A: h^{E}(a)$$

Complexity

Algorithm elim-opt (Dechter, 1996) Non-serial Dynamic Programming (Bertele and Briochi, 1973)

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



Induced Width

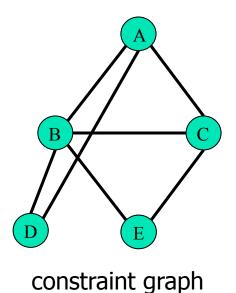
Bucket-elimination is **time** and **space**

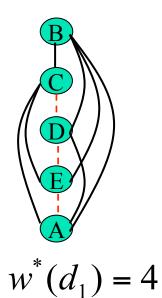
$$O(r \exp(w^*(d)))$$

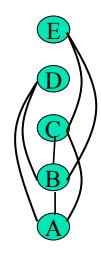
 $w^*(d)$ - the induced width of the primal graph along ordering d

r = number of functions

The effect of the ordering:



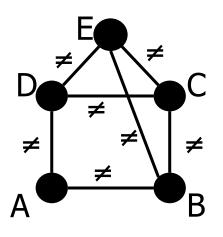


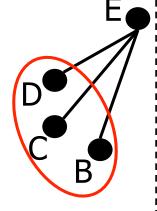


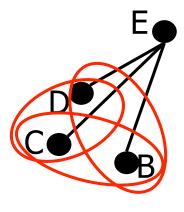
$$w^*(d_2) = 2$$

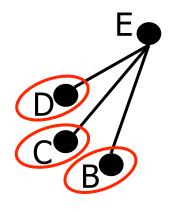
Finding smallest induced-width is hard

Directional i-consistency









 $E: E \neq D, E \neq C, E \neq B$

 $D: D \neq C, D \neq A$

 $\rightarrow R_{DCB}$

Adaptive

 $C: C \neq B$

 $B: A \neq B$

A:

d-path

 R_{DC}, R_{DB} R_{CB}

d-arc

 $egin{aligned} R_D \ R_C \ R_D \end{aligned}$

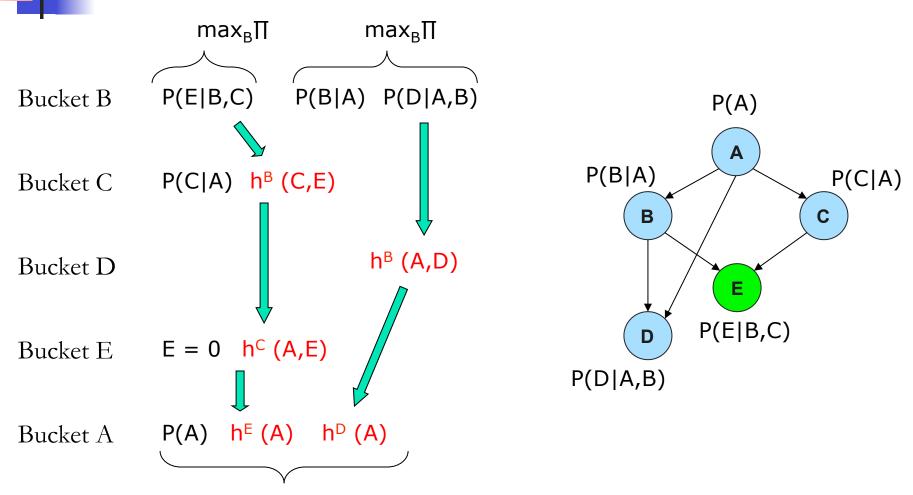
Mini-bucket approximation

Split a bucket into mini-buckets =>bound complexity

$$\begin{array}{c} \text{bucket } (\mathbf{X}) = \\ \{ \ \mathbf{h}_1, \dots, \mathbf{h}_r \ , \mathbf{h}_{r+1}, \dots, \mathbf{h}_n \ \} \\ \\ h^{\mathbf{X} = \max_{\mathbf{X}} \prod_{i=1}^{n} \mathbf{h}_i \\ \\ \mathbf{h}_1, \dots, \mathbf{h}_r \ \} \\ \\ \mathbf{g}^{\mathbf{X} = (\max_{\mathbf{X}} \prod_{i=1}^{r} \mathbf{h}_i) \cdot (\max_{\mathbf{X}} \prod_{i=r+1}^{n} \mathbf{h}_i) \\ \\ \end{pmatrix} \\ \mathbf{h}^{\mathbf{X}} \leq \mathbf{g}^{\mathbf{X}} \end{array}$$

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

Mini-Bucket Elimination



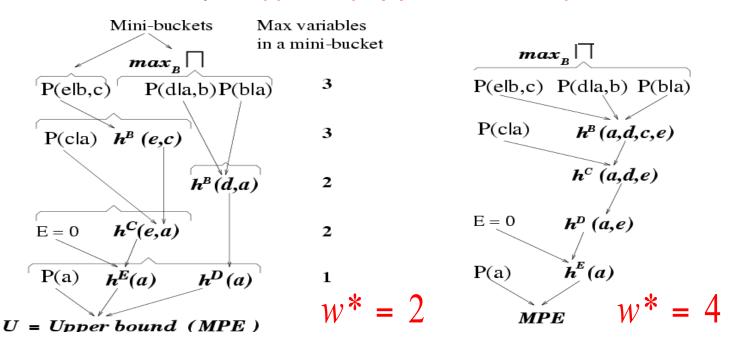
MPE* is an upper bound on MPE --U
Generating a solution yields a lower bound--L

MBE-MPE(i)

Algorithm Approx-MPE (Dechter&Rish 1997)

- Input: i max number of variables allowed in a mini-bucket
- Output: [lower bound (cost of a sub-optimal solution), upper bound]

Example: approx-mpe(3) versus elim-mpe



Properties of MBE(i)

- Complexity: O(r exp(i)) time and O(exp(i)) space.
- Yields an upper-bound and a lower-bound.
- Accuracy: determined by upper/lower (U/L) bound.
- As i increases, both accuracy and complexity increase.
- Possible use of mini-bucket approximations:
 - As anytime algorithms
 - As heuristics in search
- Other tasks: similar mini-bucket approximations for: belief updating, MAP and MEU (Dechter and Rish, 1997)

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Branch and Bound

```
procedure BRANCH-AND-BOUND
Input: A cost network \mathcal{C} = (X, D, C_h, C_s), L current upper-bound, An upper-bound
function f defined for every partial solution.
Output: Either an optimal (maximal) solution, or notification that the network is
inconsistent.
i \leftarrow 1
                                  (initialize variable counter)
D_i' \leftarrow D_i
                                  (copy domain)
While 1 \le i \le n
instantiate x_i \leftarrow \text{SELECTVALUE}
                                  (no value was returned)
If x_i is null
i \leftarrow i - 1
                                  (backtrack)
Else
i \leftarrow i + 1
                                  (step forward)
D'_i \leftarrow D_i
Endwhile
If i = 0
Return "inconsistent"
Compute C = C(x_1, ..., x_n), U \leftarrow max\{C, L\}
i \leftarrow n-1
end procedure
procedure SELECTVALUE
If i=0 return U as the solution value and the most recent assignment as solution.
While D'_i is not empty
select an element a \in D'_i having max f(\vec{a}_{i-1}, a)
and remove a from D'_i
If \langle x_i, a \rangle is consistent with \vec{a}_{i-1} and f > L, then
Return a
                                  (else prune a)
Endwhile
Return null
                                  (no consistent value)
end procedure
```

A Combinatorial Auction Example

Example 13.1.2 Consider the combinatorial auction problem. A simple approach for modeling this problem as a COP is to associate each bid b_i with a variable having two values $\{0,1\}$, where $b_i = 1$ means that the bid is selected by the auctioneer. Otherwise, it is assigned $b_i = 0$. For every two bids that share an item there is a binary constraint prohibiting the assignment of 1 to both bid variables. Therefore, the variables are: $b_1, ..., b_r$ having domains $\{0,1\}$ and the constraints are: $\forall i,j, if b_i \ and b_j$ share an item, there is a constraint R_{ij} , such that, $(b_i = 1, b_j = 1) \notin R_{ij}$. The cost functions are: for every b_i $F(b_i) = r_i$ if $b_i = 1$ and otherwise "0". The global cost function is $C = \sum_i F_i(b_i)$. The task is to find a consistent assignment to $b_1, ... b_5$ having $\max_{b_1, ... b_5} \sum_i F_i(b_i)$.

Consider a problem instance given by the following bids: $b_1 = \{1, 2, 3, 4, \}$, $b_2 = \{2, 3, 6\}$, $b_3 = \{1, 5, 4\}$, $b_4 = \{2, 8\}$, $b_5 = \{5, 6\}$ and the costs $r_1 = 8$, $r_2 = 6$, $r_3 = 5$, $r_4 = 2$, $r_5 = 2$. In this case the variables are b_1, b_2, b_3, b_4, b_5 , their domains are $\{0, 1\}$ and the constraints are $R_{12}, R_{13}, R_{14}, R_{24}, R_{25}, R_{35}$. The cost network for this problem formulation is identical to its constraint network, since all the cost components are unary. The reader can verify that an optimal solution is given by $b_1 = 0, b_2 = 1, b_3 = 1, b_4 = 0, b_5 = 0$. Namely, selecting bids b_2 and b_3 is an optimal choice with total cost of 11.

Search tree for first-choice heuristic

$$f_{fc}(\vec{a}_i) = \sum_{F_j \in C} \max_{a_{i+1},...a_n} F_j(\vec{a}_n)$$

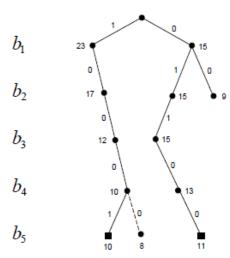


Figure 13.3: Branch and bound search space for the auction problem

Example 13.2.1 Consider the auction problem described in Example 13.1.2. Searching for a solution in the order $d = b_1, b_2, b_3, b_4, b_5$ yields the search space in Figure 13.3, traversed from left to right. The search space is highly constrained in this case. The evaluation bounding function at each node should *overestimates* its best extension for a solution. The first-choice bounding function for the root node (the empty assignment) is 23. The first solution encountered (selecting $< b_1, 1 >$ and $< b_5, 1 >$) has a cost of 10, which becomes the current global *lower bound*. The next solution encountered has the cost of 11 (when $< b_2, 1 >$ and $< b_3, 1 >$), while the rest of the variables are assigned 0). Subsequently, the partial assignment ($< b_1, 0 >, < b_2, 0 >$) is explored. Since $f_{fc}(< b_1, 0 >, < b_2, 0 >) = 9$, this upper bound is lower than 11, and therefore search can be pruned.

Bucket-Elimination for the Auction Example

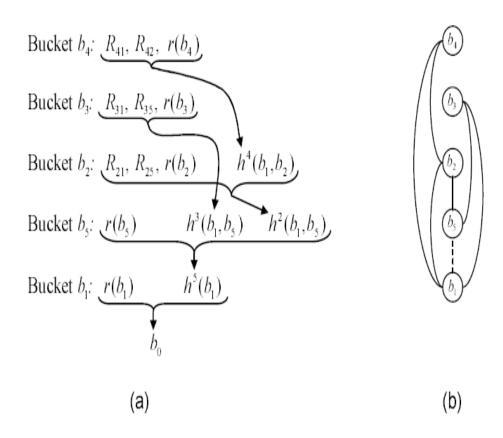


Figure 13.8: Schematic execution of elim-opt on the auction problem

Elim-OPT for auction problem

Bucket b_4 : R_{41} , R_{42} , $r(b_4)$ Bucket b_3 : R_{31} , R_{35} , $r(b_3)$ Bucket b_2 : R_{21} , R_{25} , $r(b_2)$ Bucket b_5 : $r(b_5)$ Bucket b_1 : $r(b_1)$ $h^5(b_1)$ Bucket h_1 : $h^5(b_1)$

ket b_4 . In this bucket we compute $h^4(b_1, b_2) = \max_{\{(b_4|(b_1, b_2, b_4) \in R_{41} \bowtie R_{42}\}} r(b_4)$,

$$h^4(b_1, b_2) = \begin{cases} 0 & \text{if } b_1 = 1, \text{ or } b_2 = 1\\ 2 & \text{if } b_1 = 0, b_2 = 0 \end{cases}$$

eket b_3 we compute $h^3(b_1, b_5) = \max_{\{(b_3|(b_1, b_3, b_5) \in R_{31} \bowtie R_{35}\}} r(b_3)$, yielding:

$$h^3(b_1, b_5) = \begin{cases} 0 & \text{if } b_1 = 1, \text{ or } b_5 = 1\\ 5 & \text{if } b_1 = 0, b_5 = 0 \end{cases}$$

eket b_2 , which now includes a new function, gives us: $\mathbb{E}_{\{(b_2|(b_1,b_2,b_5)\in R_{21}\bowtie R_{25}\}}(r(b_2)+h^4(b_1,b_2))$, yielding:

$$h^{2}(b_{1}, b_{5}) = \begin{cases} 0 & \text{if } b_{1} = 1, b_{5} = 1\\ 0 & \text{if } b_{1} = 1, b_{5} = 0\\ 2 & \text{if } b_{1} = 0, b_{5} = 1\\ 6 & \text{if } b_{1} = 0, b_{5} = 0 \end{cases}$$

Example MBE-opt

Example 13.4.3 Let us apply algorithm mbe-opt(2) to the auction problem along the ordering $d = b_1, b_5, b_2, b_3, b_4$. Figure 13.12 shows the resulting mini-buckets; square brackets denote the choice for partitioning.

We start with processing bucket b_4 . A possible partitioning places the constraint R_{41} in one mini-bucket and the rest in the other. We compute a constraint $R^4(b_1) = \pi_{b_1}R_{41}$, which is the universal constraint so it need not be recorded. In the second mini-bucket, we also compute $h^4(b_2) = \max_{\{(b_4)(b_4,b_2) \in R_{42}\}} r(b_4)$, yielding:

$$h^4(b_2) = \begin{cases} 0 & \text{if } b_2 = 1\\ 2 & \text{if } b_2 = 0 \end{cases}$$

Processing the first mini-bucket of b_3 , which includes only hard constraints, will also not effect the domain of b_1 . Processing the second mini-bucket of b_3 by $h^3(b_5) = \max_{\{(b_3|(b_3,b_5)\in R_{35}\}} r(b_3)$ yields:

$$h^3(b_5) = \begin{cases} 0 & \text{if } b_5 = 1\\ 5 & \text{if } b_5 = 0 \end{cases}$$

Processing the second mini-bucket of b_2 (the first mini-bucket includes a constraint whose projection is a universal constraint) by $h^2(b_5) = \max_{\{(b_2|(b_2,b_5)\in R_{25}\}}(r(b_2) + h^4(b_2))$, gives us:

$$h^2(b_5) = \begin{cases} 2 & \text{if } b_5 = 1\\ 6 & \text{if } b_5 = 0 \end{cases}$$

Processing bucket b_5 (with full buckets now) the algorithm computes $h^5 = \max_{b_5}(r(b_5) + h^2(b_5) + h^3(b_5))$, yielding:

$$h^5 = 11$$

Finally, in the bucket of b_1 the algorithm computes $h^1 = \max_{b_1}(r(b_1) + h^5)$, yielding: $h^1 = \max\{0 + 11, 8 + 11\} = 19$.

The maximal upper-bound cost is therefore 19. To compute a maximizing tuple we select in bucket b_1 the value $b_1 = 1$, which maximizes $r(b_1) + h^5$. Given $b_1 = 1$, we choose $b_5 = 0$, which maximizes the functions in bucket b_5 . Then, in bucket b_2 , we can choose only $b_2 = 0$, due to the constraint R_{12} . Likewise, the only subsequent choices are $b_3 = 0$ and $b_4 = 0$. Therefore, the cost of the generated solution is 8, yielding the interval [8,19] bounding the maximal solution.

Bucket b_4 : $[R_{41}], [R_{42}, r(b_4)]$

Bucket b_3 : $[R_{31}], [R_{35}, r(b_3)]$

Bucket b_2 : $[R_{21}], [R_{25}, r(b_2) \mid \mid h^4(b_2)]$

Bucket b_5 : $[r(b_5) || h^3(b_5), h^2(b_5)]$

Bucket $b_1: r(b_1) \parallel h^5$

Yielding: opt: $h^1 = M'$

BnB with first-cut heuristic

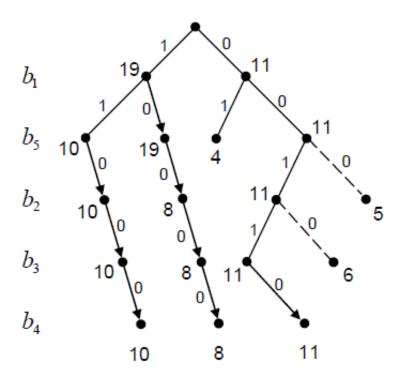
Example 13.5.4 We next demonstrate branch and bound search on the auction problem with two bounding functions. The first bounding function is first-cut f_{fc} , and the second is computed by mbe-opt(2), denoted f_{mb} . Figure 13.14 shows the search space with the two bounding functions searching along ordering b_1, b_5, b_2, b_3, b_4 . We start with f_{fc} .

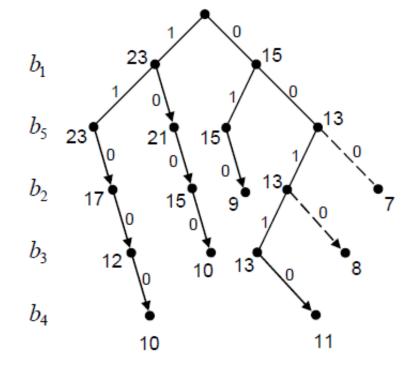
Starting with b_1 we get $f_{fc}(b_1) = r(b_1) + 15$. Thus, $f_{fc}(b_1 = 0) = 15$ and $f_{fc}(b_1 = 1) = 8 + 15 = 23$. Therefore $b_1 = 1$ is selected first. Next, the algorithm decides a value for b_5 . We get $f_{fc}(b_1 = 1, b_5 = 0) = 8 + 0 + 13 = 21$, while $f_{fc}(b_1 = 1, b_5 = 1) = 8 + 2 + 13 = 23$, consequently $b_5 = 1$ is selected. For the rest of the variables the constraints dictates $b_2 = 0, b_3 = 0, b_4 = 0$, yielding a solution with cost of 10 and a current lower bound of

L=10. The f_{fc} values are denoted next to each node. We backtrack to the closest choice node and choose the only alternative $b_5 = 0$, whose value is 21. Then, $b_2 = 0$ is the only choice due to the constraint with $b_1 = 1$. Since $f_{fc}(b_1 = 1, b_5 = 0, b_2 = 0) = 8 + 7 = 15$, pruning will not occur. The only choice for b_3 is 0, with the value 8+2=10. Since the upper bound for this node equals the lower-bound, we prune. BnB backtracks to the next choice point of $b_1 = 0$, whose bound value is (0+15=15), and so on. The next variable is b_5 . Since $f_{fc}(b_1 = 0, b_5 = 1) = 15$, and $f_{fc}(b_1 = 0, b_5 = 0) = 0 + 13 = 13$, $b_5 = 1$ is selected. Then, the only value possible for b_2 is "0" with: $f_{fc}(b_1=0,b_5=1,b_2=0)=9$. Since this upper bound is lower than the global lower bound, 10, pruning occurs and the algorithm backtracks to $b_5 = 0$. The next variable is b_2 . We get $f_{fc}(b_1 = 0, b_5 = 0, b_2 = 1) = 13$ while $f_{fc}(b_1=0,b_5=0,b_2=0)=7$. We select $b_2=1$. Subsequently, for b_3 we have the choice of $f_{fc}(b_1 = 0, b_5 = 0, b_2 = 1, b_3 = 1) = 13$, or $f_{fc}(b_1 = 0, b_5 = 0, b_2 = 1, b_3 = 0) = 8$. We select $b_3 = 1$ and are left with $b_4 = 0$, with cost of $f(b_1 = 0, b_5 = 0, b_2 = 1, b_3 = 1, b_4 = 0) = 11$. We update the global lower bound to L=11. Backtracking to the next choice point, the algorithm tries $b_3 = 0$ but its function evaluates to "8," causing another backtracking to $b_2 = 0$ with bounding value 7, causing backtracking to the root.



BnB with first-cut (b) and mini-bucket (a) heuristics





(b)

(a)

Search with MB heuristic

Let us now apply BnB with f_{mb} , which is the bounding function extracted from mbeopt(2). Based on the functions in the augmented bucket of b_1 produced by mbe-opt(2), $f_{mb}(b_1=0)=r(b_1)+h^5=8+11=19$ while $f_{mb}(b_1=1)=0+11=11$. Consequently, $b_1 = 1$ is chosen. We next evaluate $f_{mb}(b_1 = 1, b_5) = 8 + h^3(b_5) + h^2(b_5)$, yielding $f_{mb}(b_5=0)=19$ and $f_{mb}(b_5=1)=10$. Consequently, $b_5=0$ is chosen. The path is now deterministic, allowing the only choices: $b_2 = b_3 = b_4 = 0$. We end up with a solution having a cost of 8, which becomes the first global lower bound L = 8. BnB backtracks. The path is deterministic, dictating the choices $(b_2 = b_3 = b_4 = 0)$ whose bounding cost equals 10, yielding a solution with cost 10 $(b_1 = 1, b_5 = 1, b_2 = 0, b_3 = 0, b_4 = 0,)$. The global lower bound L is updated to 10. The algorithm backtracks to the next choice point, which is $(b_1 = 0)$, whose bounding cost is 11. Next, for b_5 , $f_{mb}(b_1 = 0, b_5) =$ $0 + r(b_5) + h^2(b_5) + h^3(b_5)$, yielding $f_{mb}(b_5 = 1) = 4$, which can be immediately pruned (less than 10), and $f_{mb}(b_5 = 1) = 11$. We select $b_5 = 0$. Subsequently, choosing a value for b_2 we get: $f_{mb}(b_1 = 0, b_5 = 0, b_2) = r(b_2) + h^4(b_2) + h^3(b_5)$ (note that $h^2(b_5)$ is not included since it is created in bucket b_2). This yields $f_{mb}(b_2 = 1) = 11$, while $f_{mb}(b_2 = 0) = 5$, which is pruned. The next choice for b_3 is determined using the bounding function $f_{mb}(b_1 = 0, b_5 = 0, b_2 = 1, b_3) = 6 + r(b_3) + h^4(b_2 = 1)$, yielding for $b_3 = 1$ the bound 11, while for $b_3 = 0$ the bound 6, which will be pruned. $b_3 = 1$ is selected. Subsequently, only $b_4 = 0$ is feasible and we get the best cost solution of value 11. The global lower bound, L is updated to 11 and BnB will lead to only pruned choices. We see in this example that the performance of BnB using these two bounding func-

4

Bucket-elimination for counting

Algorithm elim-count

Input: A constraint network $\mathcal{R} = (X, D, C)$, ordering d.

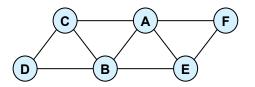
Output: Augmented output buckets including the

intermediate count functions and The number of solutions.

- 1. Initialize: Partition C (0-1 cost functions) into ordered buckets $bucket_1, \ldots, bucket_n$, We denote a function in a bucket N_i , and its scope S_i .)
- Backward: For p ← n downto 1, do
 Generate the function N^p: N^p = ∑_{Xp} ∏_{N_i∈bucket_p} N_i.
 Add N^p to the bucket of the latest variable in ⋃^j_{i=1} S_i − {X_p}.
- 3. Return the number of solutions, N^1 and the set of output buckets with the original and computed functions.

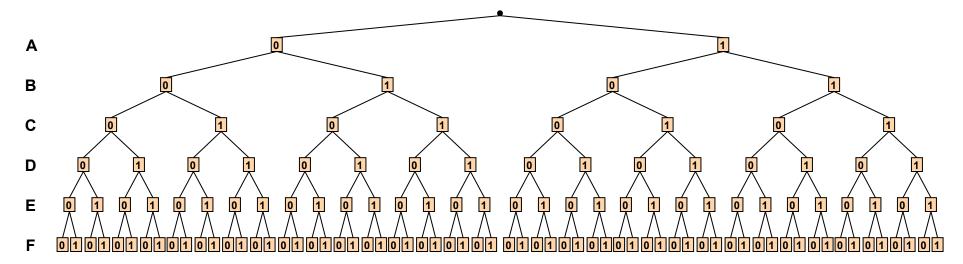


The Search Space



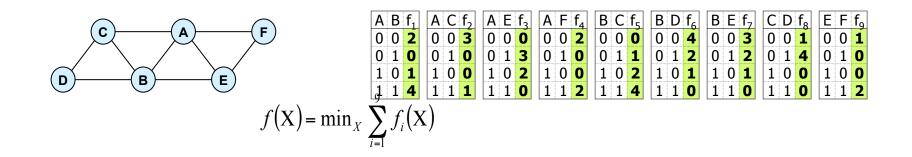
A B f ₁	A C f ₂	A E f ₃	A F f ₄	B C f ₅	BDf ₆	B E f ₇	C D f ₈	E F f _o
0 0 2	0 0 3	0 0 0	0 0 2	0 0 0	0 0 4		0 0 1	0 0 1
0 1 0	0 1 0	0 1 3	0 1 0	0 1 1	0 1 2	0 1 2	0 1 4	0 1 0
1 0 1	1 0 0	1 0 2	1 0 0	1 0 2	1 0 1	1 0 1	1 0 0	1 0 0
1 1 4	1 1 1	1 1 0	1 1 2	1 1 4	1 1 0	1 1 0	1 1 0	1 1 2

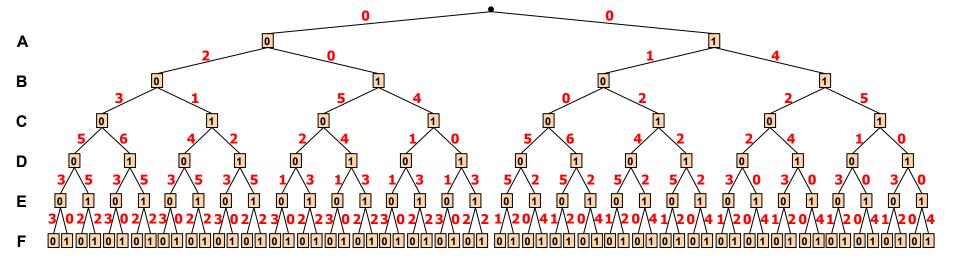
Objective function: $f(X) = \min_{X} \sum_{i=1}^{9} f_i(X)$





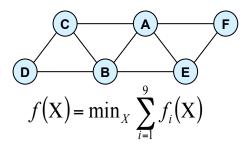
The Search Space



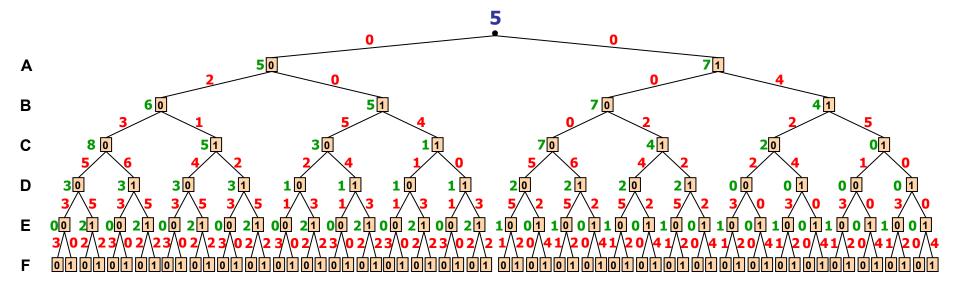


Arc-cost is calculated based on cost components.

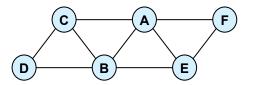




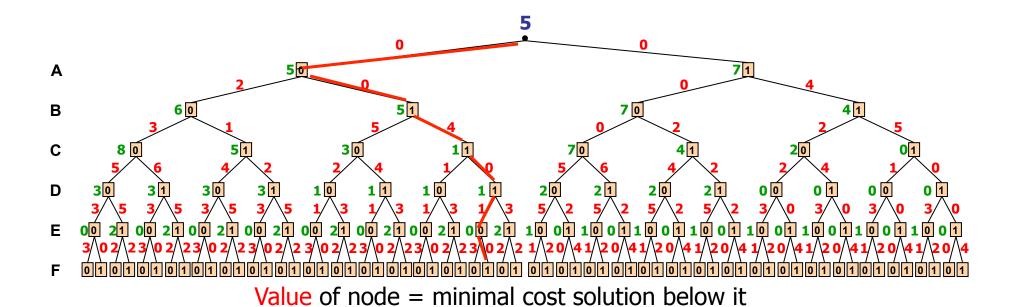
A B f ₁	$A C f_2$	A E f ₃	A F f ₄	B C f ₅	BDf_6	B E f ₇	C D f ₈	E F f ₉
0 0 2	0 0 3	0 0 0	0 0 2	0 0 0	0 0 4	0 0 3	0 0 1	0 0 1
0 1 0	0 1 0	0 1 3	0 1 0	0 1 1	0 1 2	0 1 2	0 1 4	0 1 0
1 0 1	1 0 0	1 0 2	1 0 0	1 0 2	1 0 1	1 0 1	1 0 0	1 0 0
1 1 4	1 1 1	1 1 0	1 1 2	1 1 4	1 1 0	1 1 0	1 1 0	1 1 2



An Optimal Solution



A B f ₁	$A C f_2$	A E f ₃ A 0 0 0 0	∖F f₄	B C f ₅	B D f ₆	B E f ₇	CDf 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

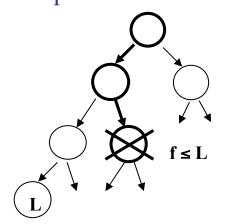


Basic Heuristic Search Schemes

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

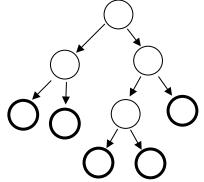
Use heuristic function $f(x^p)$ to prune the depth-first search tree. Linear space



2.Best-First Search

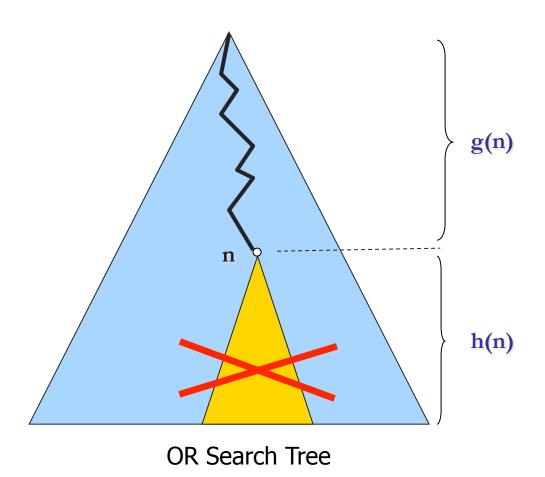
Always expand the node with the highest heuristic value $f(x^p)$.

Needs lots of memory





Classic Branch-and-Bound



Upper Bound **UB**

Lower Bound LB

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

Prune if $LB(n) \ge UB$



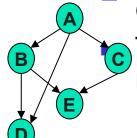
How to Generate Heuristics

- The principle of relaxed models
 - Linear optimization for integer programs
 - Mini-bucket elimination
 - Bounded directional consistency ideas



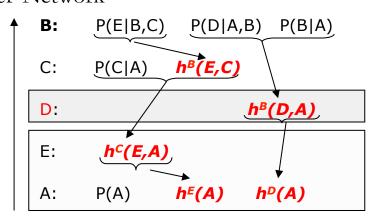
Static MBE Heuristics

Given a partial assignment xp, estimate the cost of the best extension to a full solution

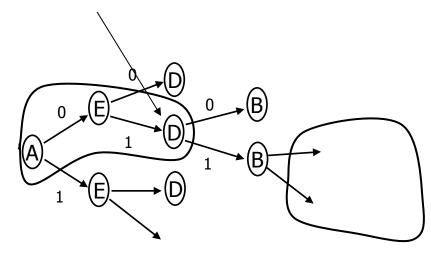


The evaluation function $f(x^p)$ can be computed using function recorded by the Mini-Bucket scheme

Belief Network



$$f(a,e,D))=g(a,e) + H(a,e,D)$$



$$f(a,e,D) = \underbrace{P(a)}_{g} + \underbrace{h^{B}(D,a) + h^{C}(e,a)}_{h-is admissible}$$

Heuristics Properties

- MB Heuristic is monotone, admissible
- Retrieved in linear time
- IMPORTANT:
 - Heuristic strength can vary by MB(i).
 - Higher i-bound ⇒ more pre-processing ⇒ stronger heuristic ⇒ less search.
- Allows controlled trade-off between preprocessing and search

4

Experimental Methodology

Algorithms

- BBMB(i) Branch and Bound with MB(i)
- BBFB(i) Best-First with MB(i)
- MBE(i)

Test networks:

- Random Coding (Bayesian)
- CPCS (Bayesian)
- Random (CSP)

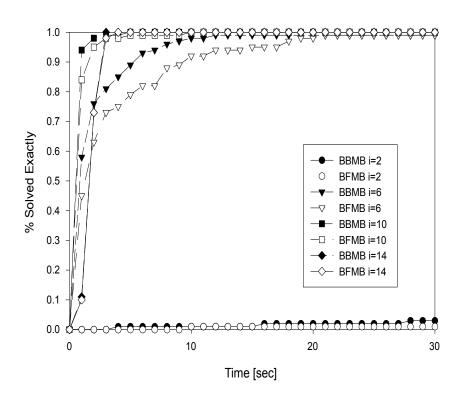
Measures of performance

- Compare accuracy given a fixed amount of time how close is the cost found to the optimal solution
- Compare trade-off performance as a function of time

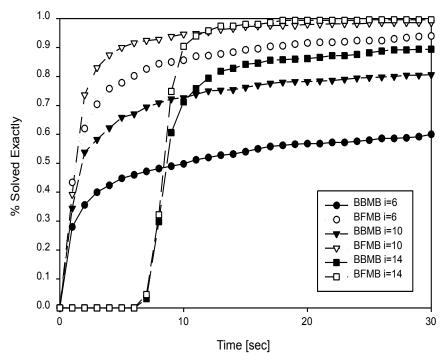


Empirical Evaluation of mini-bucket heuristics, Bayesian networks, coding

Random Coding, K=100, noise=0.28



Random Coding, K=100, noise=0.32



Max-CSP experiments

(Kask and Dechter, 2000)

	MBE	MBE	MBE	MBE	MBE	MBE	
	BBMB	BBMB	BBMB	BBMB	BBMB	BBMB	PFC-MRDAC
$\parallel T$	BFMB	BFMB	BFMB	BFMB	BFMB	BFMB	
	i=2	i=4	i=6	i=8	i=10	i=12	
	#/time	#/time	#/time	#/time	$\#/{\rm time}$	#/time	#/time
	N=10	00, K=3, C=	=200. Time	bound 1 h	r. Avg $w^*=2$	21. Sparse n	etwork.
1	70/0.03	90/0.06	100/0.32	100/2.15	100/15.1	100/116	
	90/12.5	100/0.07	100/0.33	100/2.16	100/15.1	100/116	100/0.08
	80/0.03	100/0.07	100/0.33	100/2.15	100/15.1	100/116	
2	0/-	0/-	4/0.35	20/2.28	20/15.6	24/123	
	0/-	0/-	96/644	92/41	96/69	100/125	100/757
	0/-	0/-	56/131	88/170	92/135	100/130	
3	0/-	0/-	0/-	0/-	4/14.4	4/114	
	0/-	0/-	100/996	100/326	100/94.6	100/190	100/2879
	0/-	0/-	16/597	60/462	88/344	84/216	
4	0/-	0/-	0/-	0/-	4/14.9	8/120	
	0/-	0/-	52/2228	88/1042	92/396	100/283	100/7320
	0/-	0/-	4/2934	8/540	28/365	60/866	



Dynamic MB Heuristics

- Rather than pre-compiling, the minibucket heuristics can be generated during search
- Dynamic mini-bucket heuristics use the Mini-Bucket algorithm to produce a bound for any node in the search space

(a partial assignment, along the given variable ordering)



Branch and Bound w/ Mini-Buckets

- BB with static Mini-Bucket Heuristics (s-BBMB)
 - Heuristic information is pre-compiled before search. Static variable ordering, prunes current variable
- BB with dynamic Mini-Bucket Heuristics (d-BBMB)
 - Heuristic information is assembled during search. Static variable ordering, prunes current variable
- BB with dynamic Mini-Bucket-Tree Heuristics (BBBT)
 - Heuristic information is assembled during search. Dynamic variable ordering, prunes all future variables

Empirical Evaluation

- Algorithms:
 - Complete
 - BBBT
 - BBMB
 - Incomplete
 - DLM
 - GLS
 - SLS
 - IJGP
 - IBP (coding)

Measures:

- Time
- Accuracy (% exact)
- #Backtracks
- Bit Error Rate (coding)

Benchmarks:

- Coding networks
- Bayesian Network Repository
- Grid networks (N-by-N)
- Random noisy-OR networks
- Random networks



Real World Benchmarks

				BBBT/	BBBT/	BBBT/	BBBT/			
		avg.	max	BBMB/	BBMB/	BBMB/	BBMB/	GLS	DLM	SLS
Network	# vars	dom.	dom.	IJGP	IJGP	IJGP	IJGP			
				i=2	i=4	i=6	i=8	%	%	%
				%[time]	%[time]	%[time]	%[time]	[time]	[time]	[time]
				100[0.28]	100[0.56]	-	-	15	0	90
Mildew	35	17	100	30[10.5]	95[0.18]	-	-	[30.02]	[30.02]	[30.02]
				90[3.59]	97[33.3]	-	-			
				95[1.65]	95[1.65]	95[2.32]	100[1.97]	0	0	0
Munin2	1003	5	21	95[30.3]	95[30.5]	95[31.3]	100[1.84]	[30.01]	[30.01]	[30.01]
				95[2.44]	95[5.17]	95[64.9]	-			
				90[15.2]	100[3.73]	100[2.36]	100[0.58]	10	0	0
Pigs	441	3	3	0[30.01]	60[4.85]	80[0.02]	95[0.04]	[30.02]	[30.02]	[30.02]
				80[0.31]	77[0.53]	80[1.43]	83[6.27]			
				100[0.17]	100[0.27]	100[0.21]	100[0.19]	100	100	100
CPCS360b	360	2	2	100[0.04]	100[0.03]	100[0.03]	100[0.03]	[30.02]	[30.02]	[30.02]
				100[10.6]	100[10.5]	100[9.82]	100[8.59]			

Average Accuracy and Time. 30 samples, 10 observations, 30 seconds

Empirical Results: Max-CSP

- Random Binary Problems: <N, K, C, T>
 - N: number of variables
 - K: domain size
 - C: number of constraints
 - T: Tightness

Task: Max-CSP

BBBT(i) vs BBMB(i), N=100

	$N = 100, K = 5, C = 300. w^* = 33.9. 10 instances. time = 600sec.$							
Т	i=2	i=3	i=4 BB	MB i=5	i=6	i=7	BBBT i=2	PFC-MPRDAC
	# solved	# solved	# solved	# solved	# solved	# solved	# solved	# solved
	time	time	time	time	time	time	time	time
	backtracks	backtracks	backtracks	backtracks	backtracks	backtracks	backtracks	backtracks
3	6	6	6	6	8	8	10	10
	6	6	6	5	6.8	15	7.73	0.03
	150K	150K	150K	115K	115K	8	60	750
5	2	2	2	2	3	3	10	10
	36	32	24	5.3	38	33	14.3	0.06
	980K	880K	650K	130K	870K	434K	114	1.5K
7	0	0	0	0	0	0	10 29 331	6 267 1.6M

BBBT(i) vs. BBMB(i).

Outline

Introduction

- Optimization tasks for graphical models
- Solving by inference and search

Inference

- Bucket elimination, dynamic programming
- Mini-bucket elimination, belief propagation

Search

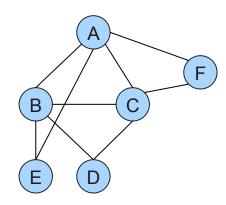
- Branch and bound and best-first
- Lower-bounding heuristics
- AND/OR search spaces

Hybrids of search and inference

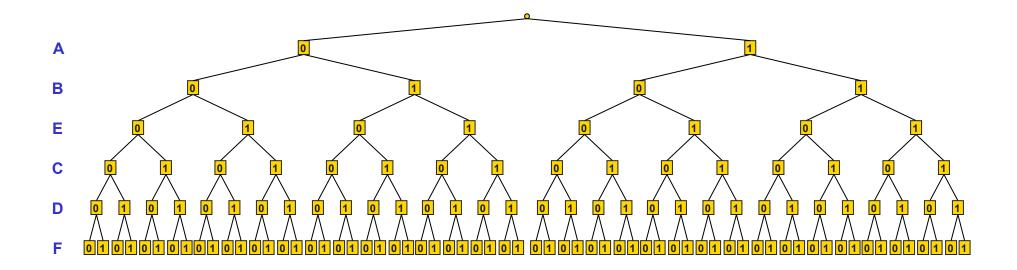
- Cutset decomposition
- Super-bucket scheme



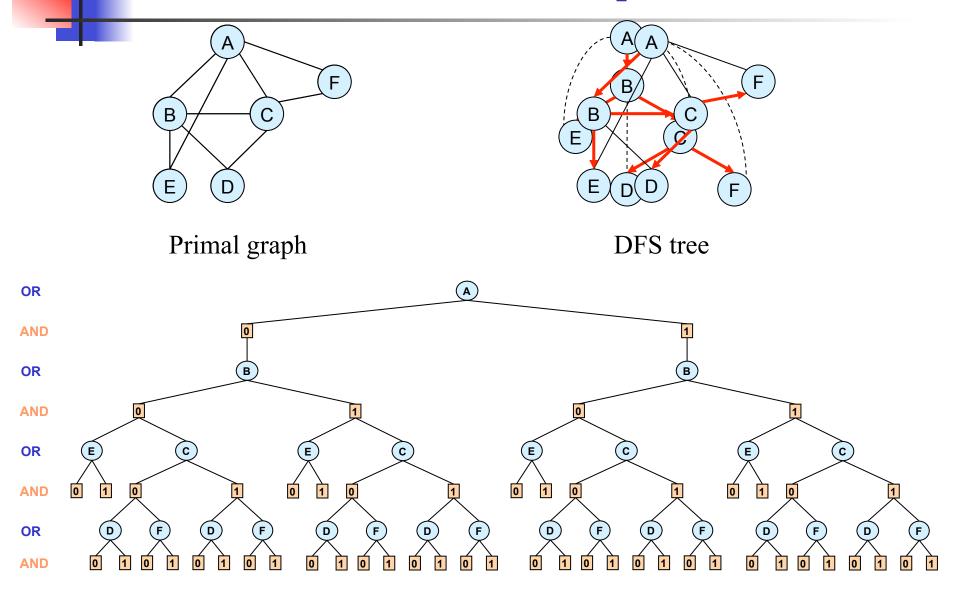
Classic OR Search Space

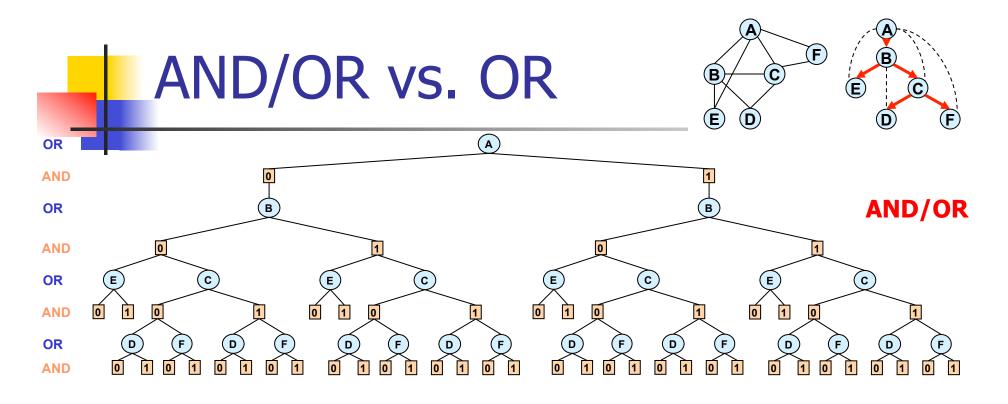


Ordering: A B E C D F

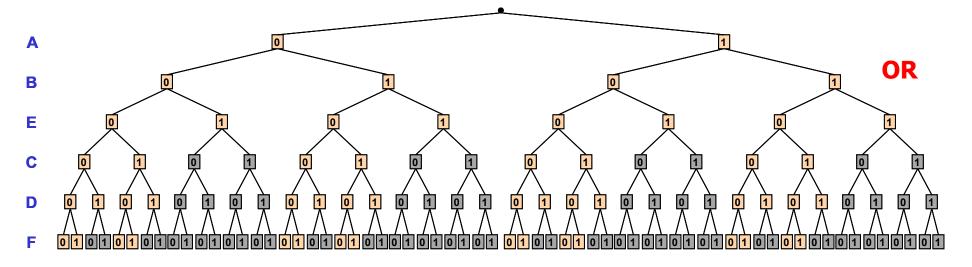


AND/OR Search Space





AND/OR size: exp(4), OR size exp(6)



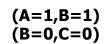
OR space vs. AND/OR space

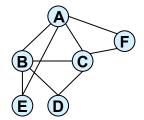
widt	heigh		OR space		AND/OR space			
h	t	Time (sec.)	Nodes	Backtracks	Time (sec.)	AND nodes	OR nodes	
5	10	3.154	2,097,150	1,048,575	0.03	10,494	5,247	
4	9	3.135	2,097,150	1,048,575	0.01	5,102	2,551	
5	10	3.124	2,097,150	1,048,575	0.03	8,926	4,463	
4	10	3.125	2,097,150	1,048,575	0.02	7,806	3,903	
5	13	3.104	2,097,150	1,048,575	0.1	36,510	18,255	

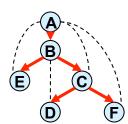
Random graphs with 20 nodes, 20 edges and 2 values per node.

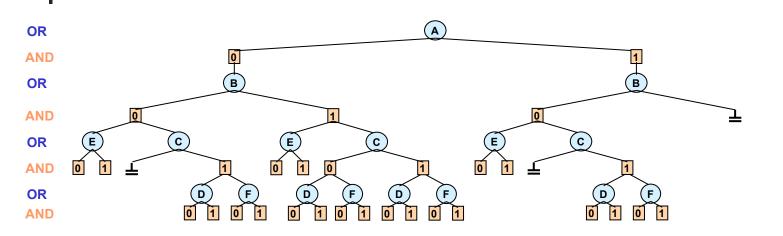


AND/OR vs. OR

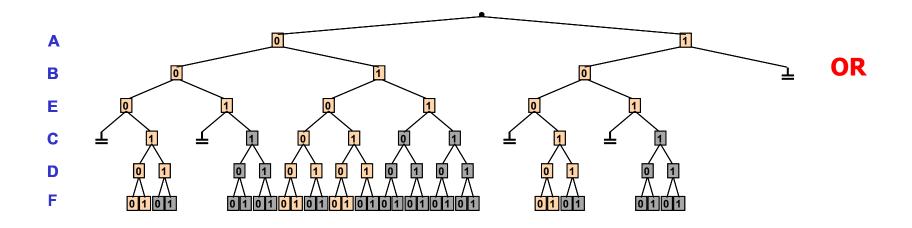






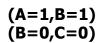


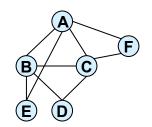
AND/OR

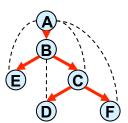


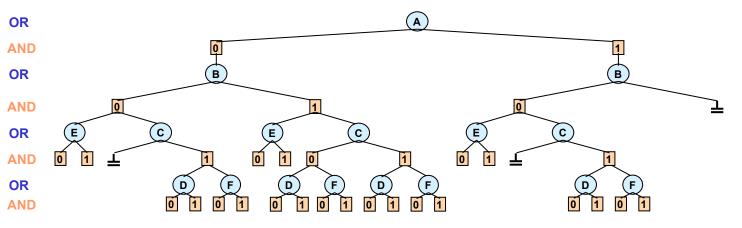


AND/OR vs. OR



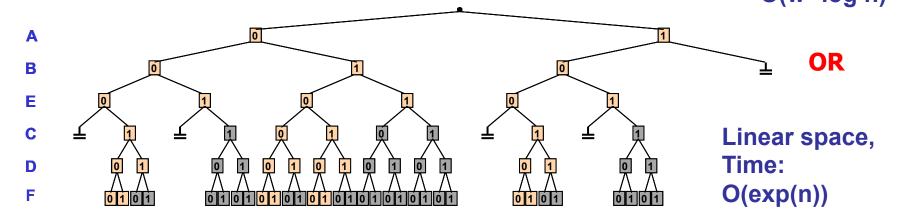




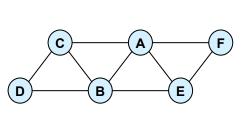


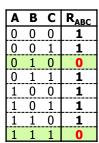
AND/OR

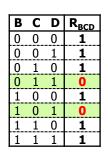
Space: linear Time: O(exp(m)) O(w* log n)

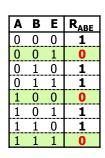


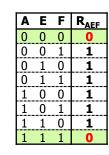
#CSP - AND/OR Search Tree

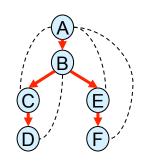


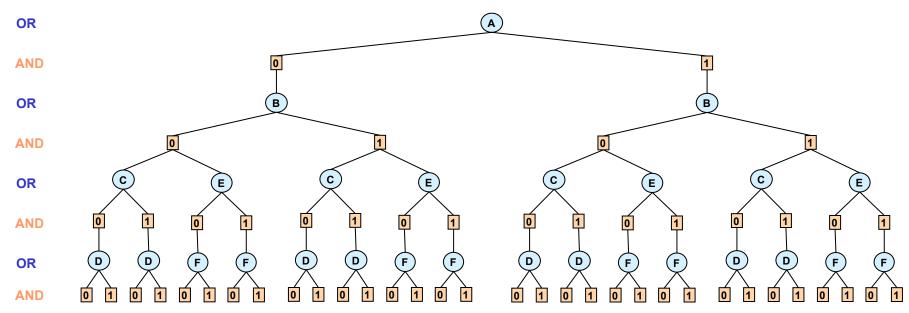












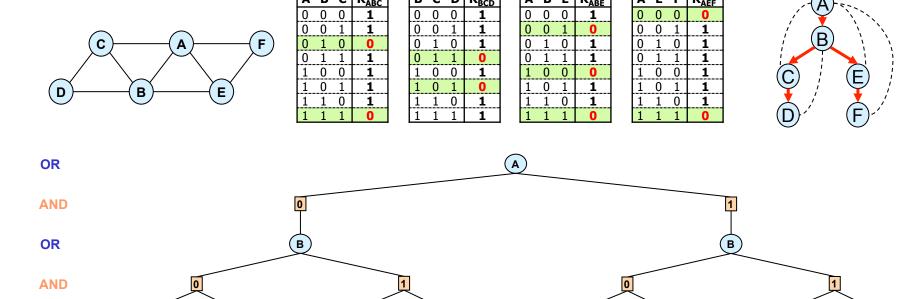
OR

AND

OR

AND

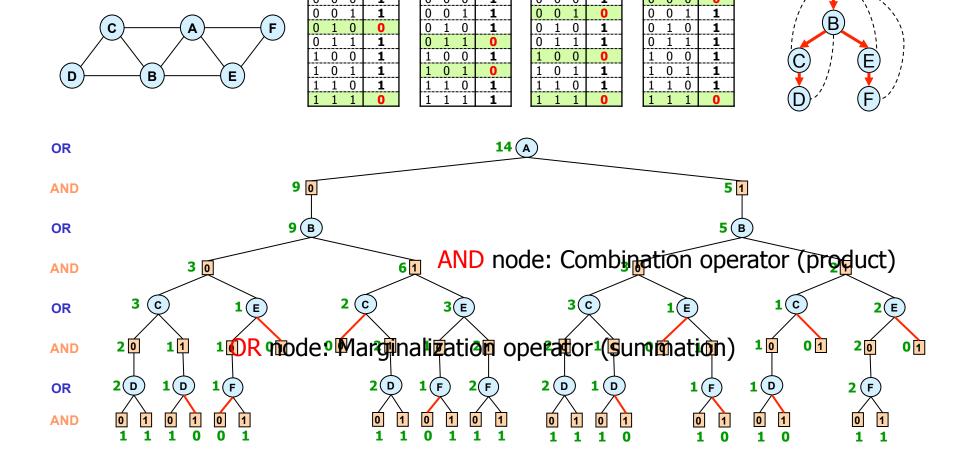
#CSP - AND/OR Search Tree



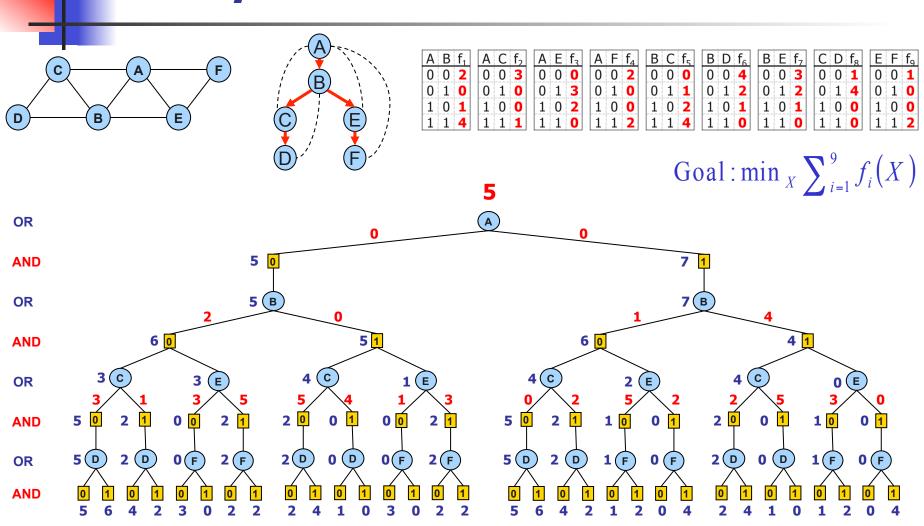
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#CSP – AND/OR Tree DFS

A E F R_{AEF}



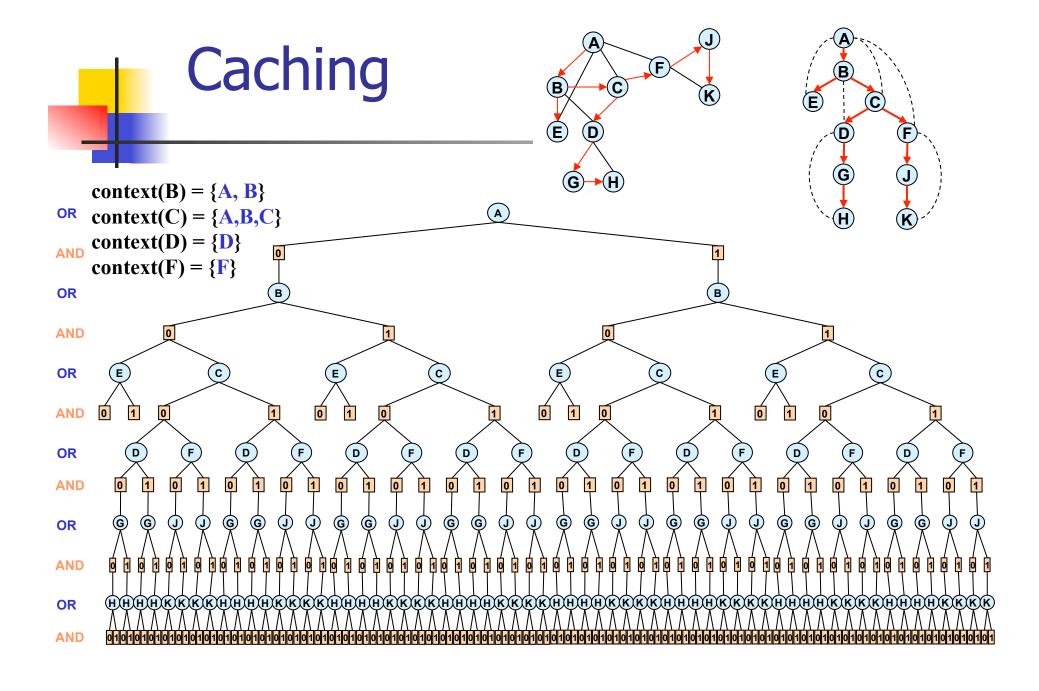
AND/OR Tree Search for COP

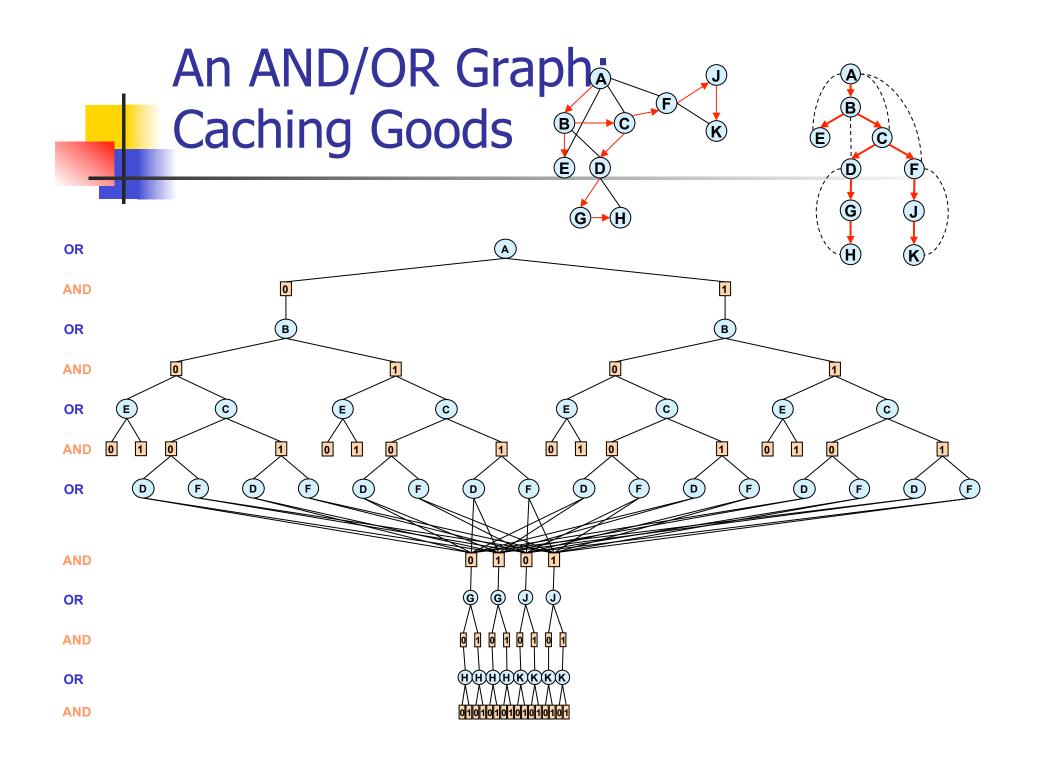


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Summary of AND/OR Search Trees

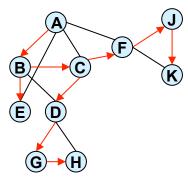
- Based on a backbone pseudo-tree
- A solution is a subtree
- Each node has a value cost of the optimal solution to the subproblem (computed recursively based on the values of the descendants)
- Solving a task = finding the value of the root node
- AND/OR search tree and algorithms are ([Freuder & Quinn85], [Collin, Dechter & Katz91], [Bayardo & Miranker95])
 - Space: O(n)
 - Time: O(exp(m)), where m is the depth of the pseudo-tree
 - Time: O(exp(w* log n))
 - BFS is time and space O(exp(w* log n)

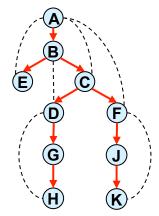




Context-based Caching

- Caching is possible when context is the same
- context = parent-separator set in induced pseudograph
 - = current variable + parents connected to subtree below





$$context(B) = \{A, B\}$$

$$context(c) = \{A,B,C\}$$

$$context(D) = \{D\}$$

$$context(F) = \{F\}$$

Complexity of AND/OR Graph

- Theorem: Traversing the AND/OR search graph is time and space exponential in the induced width/tree-width.
- If applied to the OR graph complexity is time and space exponential in the path-width.

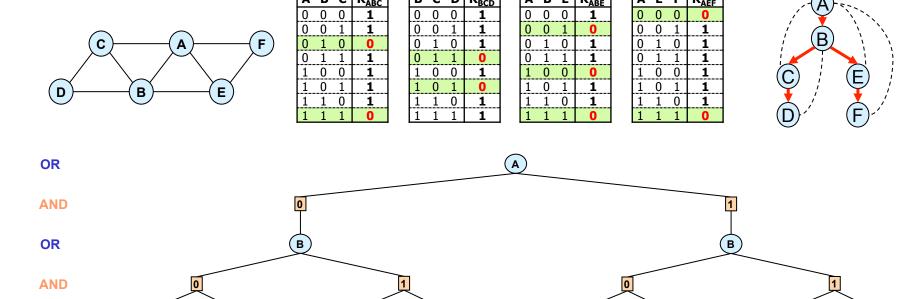
OR

AND

OR

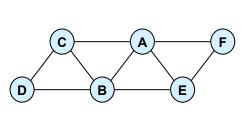
AND

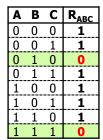
#CSP - AND/OR Search Tree



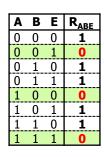
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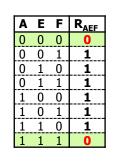
#CSP - AND/OR Tree DFS

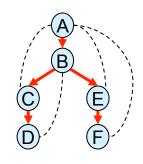


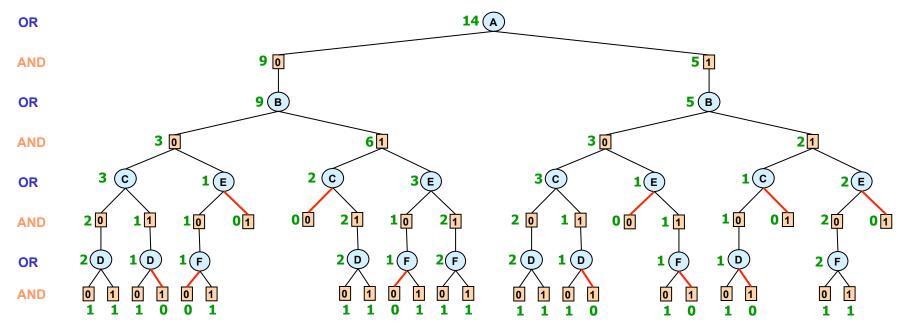


В	С	D	R _{BCD}
0	0	0	1
0	0	1	1
0	1	0	1
0	1	1	0
1	0	0	1
1	0	1	0
1	1	0	1
1	1	1	1



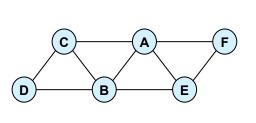


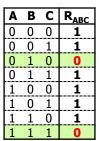


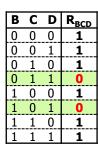


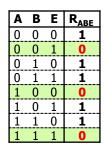
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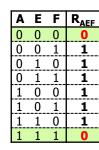
#CSP – AND/OR Search Graph (Caching Goods)

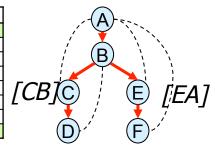


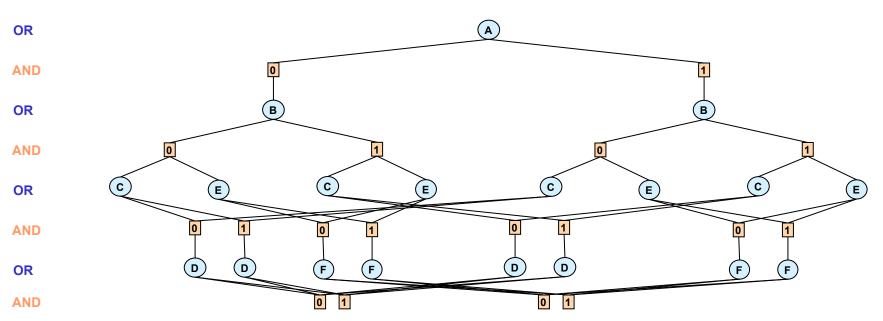






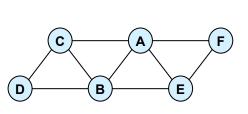


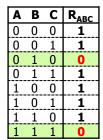


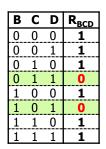


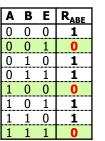


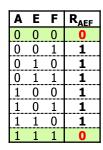
#CSP – AND/OR Search Graph (Caching Goods)

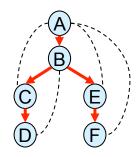


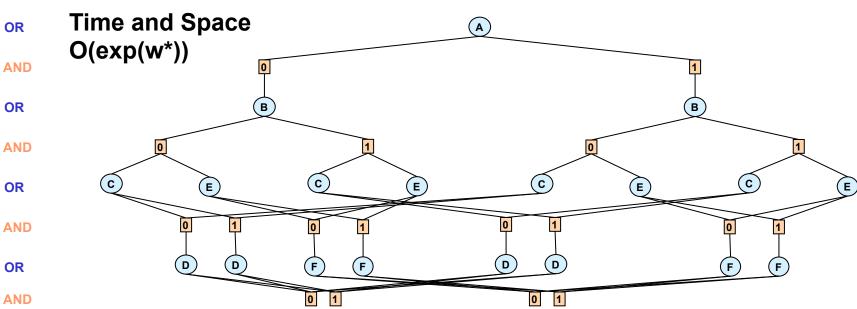








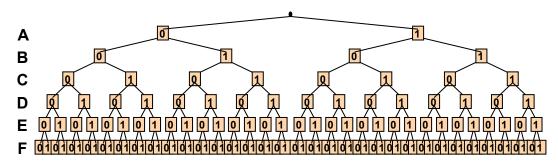




Space O(exp(sep-w*))

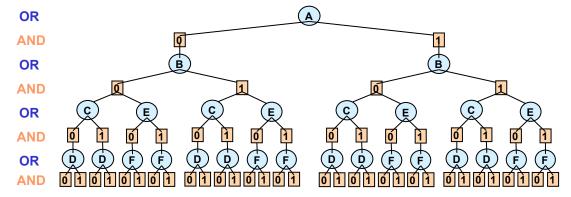


All Four Search Spaces



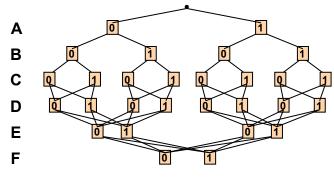
Full OR search tree

126 nodes



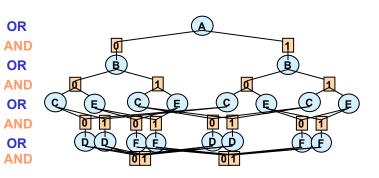
Full AND/OR search tree

54 AND nodes



Context minimal OR search graph

28 nodes



Context minimal AND/OR search graph

18 AND nodes

4

AND/OR vs. OR DFS algorithms

```
    k = domain size
    m = pseudo-tree depth
    n = number of variables
    w*= induced width
    pw*= path width
```

AND/OR tree

Space: O(n)

■ Time: O(n k^m)

 $O(n k^{w* log n})$

(Freuder85; Bayardo95; Darwiche01)

OR tree

Space: O(n)

■ Time: O(kⁿ)

AND/OR graph

Space: O(n kw*)

■ Time: O(n k^{w*})

OR graph

Space: O(n kpw*)

■ Time: O(n k^{pw*})



Searching AND/OR Graphs

- AO(i): searches depth-first, cache i-context
 - i = the max size of a cache table (i.e. number of variables in a context)

i=0 i=w*

Space: O(n) Space: O(exp w*)

Time: O(exp(w* log n)) Time: O(exp w*)

AO(i) time complexity?

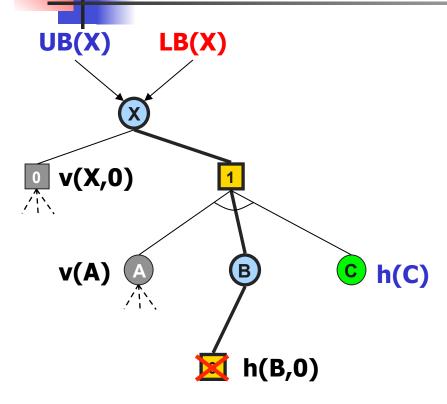


AND/OR Branch-and-Bound (AOBB)

- Associate each node n with a static heuristic estimate h(n) of v(n)
 - h(n) is a lower bound on the value v(n)
- For every node **n** in the search tree:
 - ub(n) current best solution cost rooted at n
 - lb(n) lower bound on the minimal cost at n

4

Lower/Upper Bounds



$$UB(X) = best cost below X (i.e. v(X,0))$$

$$LB(X) = LB(X,1)$$

$$LB(X,1) = I(X,1) + v(A) + h(C) + LB(B)$$

$$LB(B) = LB(B,0)$$

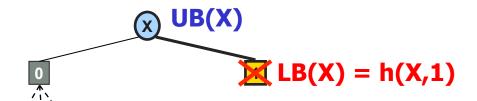
$$LB(B,0) = h(B,0)$$

Prune below AND node (B_r0) if $LB(X) \ge UB(X)$



Shallow/Deep Cutoffs

Prune if $LB(X) \ge UB(X)$



Shallow cutoff

UB(X) LB(X)

Reminiscent of **Minimax** shallow/deep cutoffs

Deep cutoff



- Traverses the AND/OR search tree in a depth-first manner
- Lower bounds computed based on heuristic estimates of nodes at the frontier of search, as well as the values of nodes already explored
- Prunes the search space as soon as an upper-lower bound violation occurs

Heuristics for AND/OR

- In the AND/OR search space h(n) can be computed using any heuristic. We used:
 - Static Mini-Bucket heuristics
 - Dynamic Mini-Bucket heuristics
 - Maintaining FDAC [Larrosa & Schiex03]
 (full directional soft arc-consistency)

Empirical Evaluation

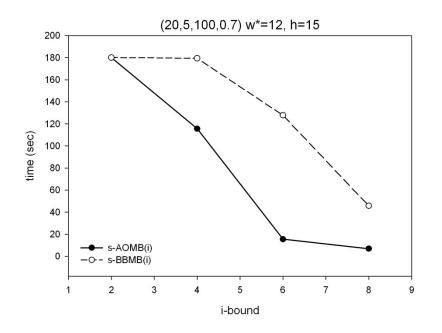
- Tasks
 - Solving WCSPs
 - Finding the MPE in belief networks
- Benchmarks (WCSP)
 - Random binary WCSPs
 - RLFAP networks (CELAR6)
 - Bayesian Networks Repository
- Algorithms
 - s-AOMB(i), d-AOMB(i), AOMFDAC
 - s-BBMB(i), d-BBMB(i), BBMFDAC
 - Static variable ordering (dfs traversal of the pseudo-tree)



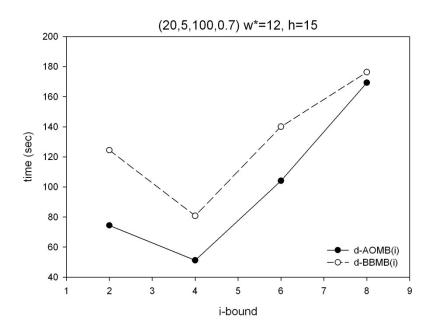
Random Binary WCSPs

(Marinescu and Dechter, 2005)

S-AOMB vs S-BBMB



D-AOMB vs D-BBMB



Random networks with n=20 (number of variables), d=5 (domain size), c=100 (number of constraints), t=70% (tightness). Time limit 180 seconds.

AO search is superior to OR search

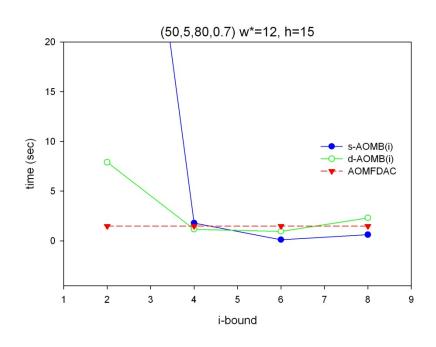


Random Binary WCSPs (contd.)



(20,5,100,0.7) w*=12, h=15 180 160 140 120 100 time (sec) d-AOMB(i) 80 60 40 20 i-bound

sparse



n=20 (variables), d=5 (domain size), n=50 (variables), d=5 (domain size), c=100 (constraints), t=70% (tightness) c=80 (constraints), t=70% (tightness)

AOMB for large i is competitive with AOMFDAC

Resource Allocation

Radio Link Frequency Assignment Problem (RLFAP)

Instance	ВВМ	DAC	AOMFDAC		
mstance	time (sec)	nodes	time (sec)	nodes	
CELAR6-SUB0	2.78	1,871	1.98	435	
CELAR6-SUB1	2,420.93	364,986	981.98	180,784	
CELAR6-SUB2	8,801.12	19,544,182	1,138.87	175,377	
CELAR6-SUB3	38,889.20	91,168,896	4,028.59	846,986	
CELAR6-SUB4	84,478.40	6,955,039	47,115.40	4,643,229	

CELAR6 sub-instances

AOMFDAC is superior to **ORMFDAC**

Bayesian Networks Repository

Network	Algorithm	i=2		i=3		i=4		i=5	
(n,d,w*,h)		time	nodes	time	nodes	time	nodes	time	nodes
	s-AOMB(i)	-	8.5M	-	7.6M	46.22	807K	0.563	9.6K
Barley	s-BBMB(i)	-	16M	-	18M	-	17M	-	14M
(48,67,7,17)	d-AOMB(i)	-	79K	136.0	23K	12.55	667	45.95	567
	d-BBMB(i)	-	2.2M	-	1M	346.1	76K	-	86K
	s-AOMB(i)	57.36	1.2M	12.08	260K	7.203	172K	1.657	43K
Munin1	s-BBMB(i)	-	8.5M	-	9M	-	10M	-	8M
(189,21,11,24)	d-AOMB(i)	66.56	185K	12.47	8.1K	10.30	1.6K	11.99	523
	d-BBMB(i)	-	405K	-	430K	-	235K	14.63	917
	s-AOMB(i)	-	5.9M	-	4.9M	1.313	17K	0.453	6K
Munin3	s-BBMB(i)	-	1.4M	-	1.2M	-	316K	-	1.5M
(1044,21,7,25)	d-AOMB(i)	-	2.3M	68.64	58K	3.594	5.9K	2.844	3.8K
	d-BBMB(i)	-	33K	-	125K	-	52K	-	31K

Time limit 600 seconds

available at http://www.cs.huji.ac.il/labs/compbio/Repository

Static AO is better with accurate heuristic (large i)

Outline

Introduction

- Optimization tasks for graphical models
- Solving by inference and search

Inference

- Bucket elimination, dynamic programming
- Mini-bucket elimination, belief propagation

Search

- Branch and bound and best-first
- Lower-bounding heuristics
- AND/OR search spaces
 - Searching trees
 - Searching graphs

Hybrids of search and inference

- Cutset decomposition
- Super-bucket scheme

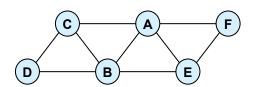


From Searching Trees to Searching Graphs

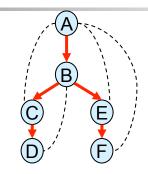
- Any two nodes that root identical subtrees/ subgraphs can be merged
- Minimal AND/OR search graph: closure under merge of the AND/OR search tree
 - Inconsistent sub-trees can be pruned too.
 - Some portions can be collapsed or reduced.



AND/OR Search Graph

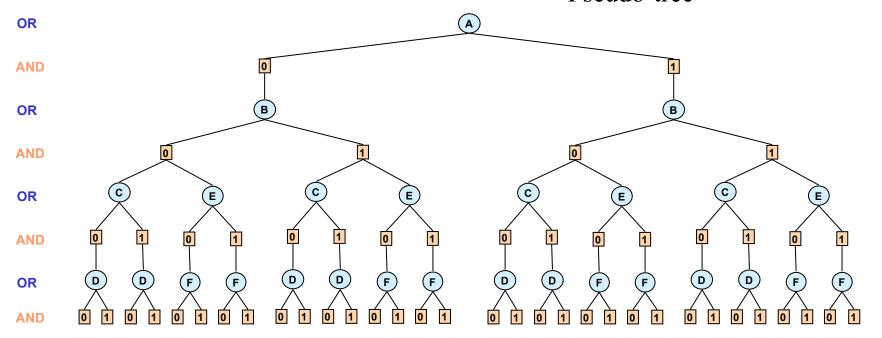


Primal graph



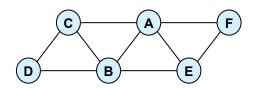
context(A) = {A}
context(B) = {B,A}
context(C) = {C,B}
context(D) = {D}
context(E) = {E,A}
context(F) = {F}

Pseudo-tree

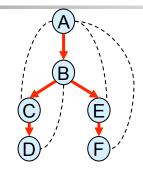




AND/OR Search Graph

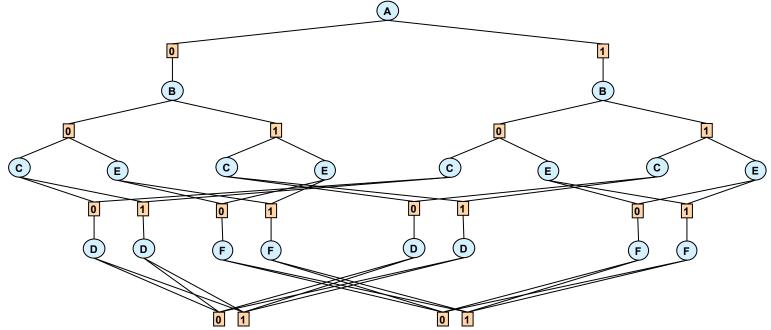


Primal graph



context(A) = {A}
context(B) = {B,A}
context(C) = {C,B}
context(D) = {D}
context(E) = {E,A}
context(F) = {F}

Pseudo-tree



AND

OR

OR

AND

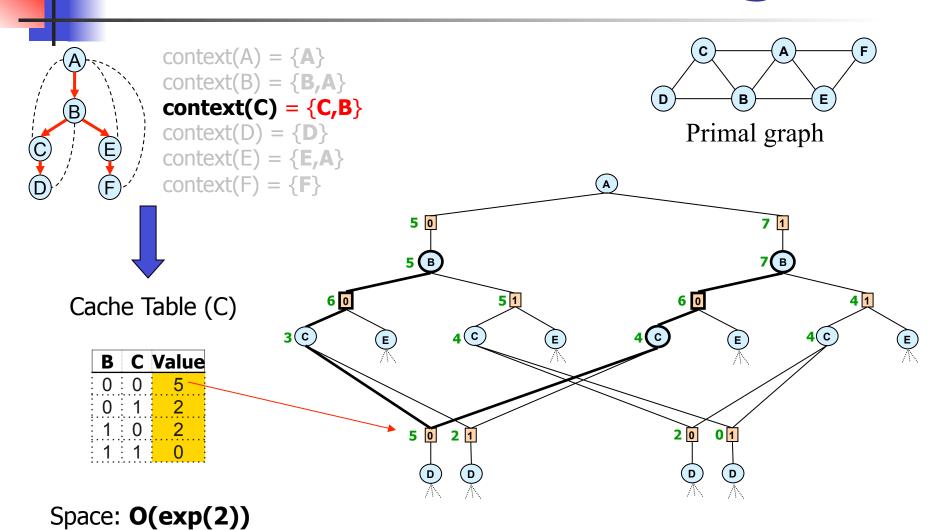
OR

AND

OR

AND

Context-based caching





Searching AND/OR Graphs

- AO(j): searches depth-first, cache j-context
 - j = the max size of a cache table (i.e. number of variables in a context)

Space: O(n) Space: O(exp w*)

Time: O(exp(w* log n)) Time: O(exp w*)

AO(j) time complexity?