AND/OR Branch-and-Bound for Graphical Models

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Abstract

The paper presents and evaluates the power of a new framework for optimization in graphical models, based on AND/OR search spaces. The virtue of the AND/OR representation of the search space is that its size may be far smaller than that of a traditional OR representation. We develop our work on *Constraint Optimization Problems* (COP) and introduce a new generation of depth-first Branch-and-Bound algorithms that explore an AND/OR search space and use static and dynamic mini-bucket heuristics to guide the search. We focus on two optimization problems, solving Weighted CSPs (WCSP) and finding the Most Probable Explanation (MPE) in belief networks. We show that the new AND/OR approach improves considerably over the classic OR space, on a variety of benchmarks including random and real-world problems. We also demonstrate the impact of different lower bounding heuristics on Branch-and-Bound exploring AND/OR spaces.

1 Introduction

Graphical models such as constraint networks and belief networks have become a powerful representation framework for reasoning with deterministic and probabilistic information. These models use graphs to capture conditional independencies between variables, allowing a concise representation of the knowledge as well as efficient graph-based query processing algorithms.

Optimization tasks such as finding the most likely state of a belief network or finding a solution that violates the least number of constraints in a constraint network are all instances of *Constraint Optimization Problems* (COP). They are typically tackled with either *search* or *inference* algorithms. Search methods (e.g. depth-first Branch-and-Bound, best-first search) are time exponential in the number of variables and can operate in polynomial space. Inference algorithms (e.g. variable elimination, tree-clustering) are time and space exponential in a topological parameter called *tree width*. If the tree width is large, the high space complexity makes the latter methods impractical.

In this paper we focus on search. In contrast to inference algorithms, search algorithms are less sensitive to the graph-model structure because they traverse a structure-blind search space. To overcome this problem the idea of AND/OR search spaces was introduced in the past year, and was shown to vividly display independencies encoded in the underlying graphical model [Dechter and Mateescu, 2004]. In this paper we develop *AND/OR Branch-and-Bound* (AOBB), a general algorithm for solving COPs, which explores the AND/OR search tree in a *depth-first* manner. Its efficiency depends on its guiding heuristic functions. In the past, a class of partitioning-based heuristic functions, based on the Mini-Bucket approximation and known as *static mini-bucket heuristics* was shown to be powerful for optimization problems [Kask and Dechter, 2001]. We take the idea one step further and introduce *dynamic mini-bucket heuristics*, which are computed dynamically at each node of the search tree. Both schemes are parameterized by the Mini-Bucket i-bound, which allows for a controllable trade-off between preprocessing and search.

We apply the AND/OR algorithms to two common optimization problems: solving Weighted CSPs [Bistarelli *et al.*, 1997] and finding the Most Probable Explanation (MPE) in belief networks [Pearl, 1988]. We experiment with both random models and real-world benchmarks. Our results show conclusively that the new AND/OR Branch-and-Bound algorithms improve dramatically over traditional OR ones, especially when the heuristic estimates are inaccurate and the algorithms rely primarily on search rather than on pruning.

2 Background

A finite *Constraint Optimization Problem* (COP) is a six-tuple $\mathcal{P} = \langle \mathcal{X}, \mathcal{D}, \mathcal{F}, \otimes, \Downarrow, Z \rangle$, where $\mathcal{X} = \{X_1, ..., X_n\}$ is a set of variables, $\mathcal{D} = \{D_1, ..., D_n\}$ is a set of finite domains and $\mathcal{F} = \{f_1, ..., f_m\}$ is a set of constraints. Constraints can be either *soft* (cost functions) or *hard* (sets of allowed tuples). Without loss of generality we assume that hard constraints are represented as (bi-valued) cost functions. Allowed and forbidden tuples have cost 0 and ∞, respectively. The scope of function f_i, denoted $scope(f_i) \subseteq \mathcal{X}$, is the set of arguments of f_i. The operators $\otimes$ and $\Downarrow$ can be defined using the semi-ring framework [Bistarelli *et al.*, 1997], but in this paper we assume that: $\otimes_i f_i$ is a *combination* operator, $\otimes_i f_i \in \{\prod_i f_i, \sum_i f_i\}$ and $\Downarrow_Y f$ is an *elimination* operator, $\Downarrow_Y f \in \{max_{S-Y} f, min_{S-Y} f\}$, where S is the scope of function f and $Y \subseteq \mathcal{X}$. The scope of $\Downarrow_Y f$ is Y.

An optimization task is defined by $g(Z) = \Downarrow_Z \otimes_{i=1}^{m} f_i$, where $Z \subseteq \mathcal{X}$. A *global optimization* is the task of finding the best global cost, namely $Z = \emptyset$. For simplicity we will develop our work assuming a COP instance with *summation* and *minimization* as combination and elimination operators, and a global cost function defined by $f(\mathcal{X}) = min_{\mathcal{X}} \sum_{i=1}^{m} f_i$.

The *primal graph* of a COP instance has the variables $\mathcal{X}$ as its nodes and an arc connects any two variables that appear in the scope of the same function.

In practice, most complete COP solvers follow a *depth-first Branch-and-Bound* strategy which maintains an *upper bound*, the best solution cost found so-far, and a *lower bound* on the optimal extension of the current assignment. Value pruning occurs as soon as the lower bound exceeds the upper bound.

3 AND/OR Search Spaces

The usual way to do search (i.e. *OR search*) is to instantiate variables in turn, following a static/dynamic linear ordering. This process defines a search tree (i.e. *OR tree*), whose nodes represent states in the space of partial assignments.

One way to exploit the independencies encoded by the graphical model is to introduce AND nodes into the search space, which will decompose the problem into separate subproblems. In the past year, [Dechter and Mateescu, 2004] introduced the concept of AND/OR search spaces for constraint networks, belief networks, and for graphical models in general. The AND/OR search space is defined using a back-bone *pseudo-tree* arrangement of the primal graph.

DEFINITION **1 (pseudo-tree)** *Given the primal graph G of a COP instance $\mathcal{P}$, a* pseudo-tree *is a rooted tree with the same set of vertices as G and has the property that adjacent vertices from G must be in the same branch of the rooted tree [Freuder and Quinn, 1985].*

DEFINITION **2 (AND/OR search tree)** *Given a COP instance $\mathcal{P}$, its primal graph G and a pseudo-tree T of G, the associated* AND/OR search tree $S_T(\mathcal{P})$ *has alternating levels of OR nodes and AND nodes. The OR nodes are labeled X_i and correspond to the variables. The AND nodes are labeled $\langle X_i, a\rangle$ and correspond to value assignments in the domains of the variables. The* root *of the AND/OR search tree is an OR node, labeled with the root of T. The children of an OR node X_i are AND nodes labeled with assignments $\langle X_i, a\rangle$, consistent along the path from the root. The children of an AND node $\langle X_i, a\rangle$ are OR nodes labeled with the children of variable X_i in T. The* path *of a node $n \in S_T$, denoted $Path_{S_T}(n)$, is the path from the the root of S_T to n, and corresponds to a partial value assignment to all variables along the path.*

A *solution subtree* Sol_{S_T} of S_T is an AND/OR subtree such that:(i) it contains the root of S_T;(ii) if a nonterminal AND node $n \in S_T$ is in Sol_{S_T} then all of its children are in Sol_{S_T};(iii) if a nonterminal OR node $n \in S_T$ is in Sol_{S_T} then exactly one of its children is in Sol_{S_T}.

Example 1 *Consider the graphical model in Figure 1(a) (top) describing a graph coloring problem over domains {0,1}. An AND/OR search tree based on the pseudo-tree in Figure 1(a) (bottom), and a highlighted solution subtree are given in Figure 1(b). Observe that the AND node $\langle B, 0\rangle$[1] roots two independent subproblems, one represented by variable $\{E\}$, and the other by variables $\{C, D, F\}$.*

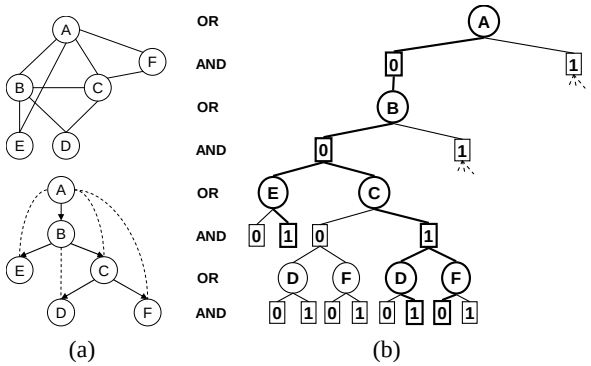


Figure 1: An AND/OR search tree.

THEOREM **1 ([Dechter and Mateescu, 2004])** *Given a COP instance $\mathcal{P}$ and a pseudo-tree T, its AND/OR search tree S_T is sound and complete (contains all and only solutions) and its size is $O(n \cdot exp(m))$, where m is the depth of the pseudo-tree.*

Any search algorithm that traverses the AND/OR search tree in a depth-first manner is guaranteed to have a time complexity exponential in the depth of the pseudo-tree and can operate in linear space. In contrast, the time complexity of search algorithms exploring traditional OR search trees is exponential in the number of variables. The arcs in S_T are annotated by appropriate *labels* of the cost functions. The nodes in S_T can be associated with a *value*, accumulating the result of the computation resulted from the subtree below.

DEFINITION **3 (label)** *The* label $l(X_i, \langle X_i, a\rangle)$ *of the arc from the OR node X_i to the AND node $\langle X_i, a\rangle$ is defined as the sum of all the cost functions values for which variable X_i is contained in their scope and whose scope is fully assigned along $Path_{S_T}(\langle X_i, a\rangle)$.*

DEFINITION **4 (value)** *The* value $v(n)$ *of a node $n \in S_T$, is defined recursively as follows: (i) if $n = \langle X_i, a\rangle$ is a terminal AND node then $v(n) = l(X_i, \langle X_i, a\rangle)$; (ii) if $n = \langle X_i, a\rangle$ is an internal AND node then $v(n) = l(X_i, \langle X_i, a\rangle) + \sum_{n' \in succ(n)} v(n')$; (iii) if $n = X_i$ is an internal OR node then $v(n) = min_{n' \in succ(n)} v(n')$, where $succ(n)$ are the children of n in S_T.*

Clearly, the value of each node can be computed recursively, from leaves to root. We can show that:

PROPOSITION **1** *Given an AND/OR search tree S_T of a COP instance $\mathcal{P} = \langle \mathcal{X}, \mathcal{D}, \mathcal{F}, +, min\rangle$, the value function $v(n)$ is the minimal cost solution to the subproblem rooted at n, subject to the current variable instantiation along the path from root to n. If n is the root of S_T, then $v(n)$ is the minimal cost solution to $\mathcal{P}$.*

Therefore, we can traverse the AND/OR search tree in a depth-first manner to compute the value of the root. This

[1] In the figure we only denote the value. $\langle B, 0\rangle$ is written as $\boxed{0}$ child of B.

approach would require linear space, storing only the current partial solution subtree. The algorithm expands alternating levels of OR and AND nodes, periodically evaluating the value function of the nodes along the current path. It terminates when the root node is evaluated with the optimal cost.

4 AND/OR Branch and Bound

If each node n at the search frontier is assigned a *heuristic lower-bound estimate* $h(n)$ of $v(n)$, then we can calculate the most promising extension of the current partial solution subtree and prune the portion of the search space that becomes irrelevant, as part of a Branch-and-Bound scheme. We call $h(n)$ a *static* heuristic function.

4.1 Lower Bounds on Partial Solution Trees

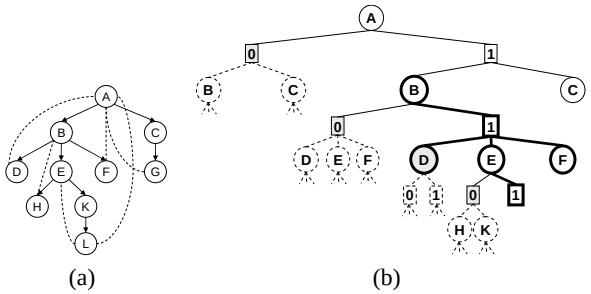
At any stage of the search, the current partial solution is a *partial solution subtree*, denoted $\mathcal{PST}$. By the nature of the search process, $\mathcal{PST}$ must be connected, must contain the root node and will have a *frontier* containing all those nodes that were generated but not yet expanded. The leaves of $\mathcal{PST}$ are called *tip* nodes. In this section we will define a *dynamic* heuristic function of a node n relative to the current $\mathcal{PST}$, which yields a more accurate lower bound on $v(n)$ than $h(n)$. For that we introduce the notions of *active path*, its *inside* and *outside contexts* and the *active partial subtree*.

DEFINITION **5** *Given the current $\mathcal{PST}$, the* active path *$\mathcal{AP}(t)$ is the path of assignments from the root of $\mathcal{PST}$ to the current tip node t. The* inside context *$in(\mathcal{AP})$ of $\mathcal{AP}(t)$ contains all nodes that were fully evaluated and are children of nodes on $\mathcal{AP}(t)$. The* outside context *$out(\mathcal{AP})$ of $\mathcal{AP}(t)$, contains all nodes that were generated but not yet expanded and are children of the nodes on $\mathcal{AP}(t)$. The* active partial subtree *$\mathcal{APT}(n)$ rooted at a node $n \in \mathcal{AP}(t)$ contains the sub-path between n and t, and all OR children of the AND nodes on it.*

For illustration consider the partial solution subtree in Figure 2(b) based on the pseudo-tree in Figure 2(a). The active path $\mathcal{AP}(t)$ has tip node $t = \langle E, 1\rangle$, namely it is $(A = 1, B = 1, E = 1)$. The shaded nodes at the left of $\mathcal{AP}(t)$ are in $in(\mathcal{AP})$ and their corresponding subtrees have already been explored. $out(\mathcal{AP})$ includes the nodes $\{C, F\}$, which are also in the search frontier. The active partial subtree $\mathcal{APT}(B)$ is highlighted. It contains the nodes $\{B, \langle B, 1\rangle, E, \langle E, 1\rangle\}$ on $\mathcal{AP}(t)$, the OR node D from $in(\mathcal{AP})$ and the OR node F from $out(\mathcal{AP})$.

DEFINITION **6 (dynamic lower bound)** *Given an active partial tree $\mathcal{APT}(n)$, the* dynamic heuristic evaluation function *of n, $f_h(n)$, is defined recursively as follows: (i) if $\mathcal{APT}(n)$ consists only of a single node n, and if $n \in in(\mathcal{AP})$ then $f_h(n) = v(n)$ else $f_h(n) = h(n)$; (ii) if $n = \langle X_i, a\rangle$ is an AND node, having OR children $m_1, ..., m_k$ then $f_h(n) = max(h(n), l(X_i, \langle X_i, a\rangle) + \sum_{i=1}^{k} f_h(m_i))$; (iii) if $n = X_i$ is an OR node, having an AND child m, then $f_h(n) = max(h(n), f_h(m))$.*

We can prove that $f_h(n)$ is a *lower bound* on the optimal solution cost to the subproblem rooted at n, namely $f_h(n) \leq v(n)$, and also by definition $f_h(n) \geq h(n)$, indicating that the dynamic lower bound is superior to the static one.



(a) (b)

Figure 2: A partial solution subtree.

Example 2 *For the active partial subtree rooted at B in Figure 2(b), the lower bound $f_h(B)$ on $v(B)$ is computed recursively as follows: $f_h(B) = max(h(B), f_h(\langle B, 1\rangle))$, where $f_h(\langle B, 1\rangle) = max(h(\langle B, 1\rangle), l(B, \langle B, 1\rangle) + v(D) + f_h(E) + h(F))$. Similarly, $f_h(E) = max(h(E), f_h(\langle E, 1\rangle)) = max(h(E), h(\langle E, 1\rangle))$, since $f_h(\langle E, 1\rangle) = h(\langle E, 1\rangle)$.*

4.2 The Branch-and-Bound Procedure

In the AND/OR search space, we can calculate a *lower bound* on $v(n)$ of a node n on the active path, by using $f_h(n)$. In addition, we can compute an *upper bound* on $v(n)$, based on the portion of the search space below n that has already been explored. The upper bound $ub(n)$ on $v(n)$ is the current minimum cost solution subtree of the subproblem rooted at n.

In Figure 2(b), the upper bound on $v(B)$ is $ub(B) = min(\infty, v(\langle B, 0\rangle)) = v(\langle B, 0\rangle)$, and it represents the current best cost solution rooted at B. The lower bound $f_h(B)$ on $v(B)$ is calculated as seen in the previous example. If $f_h(B) \geq ub(B)$, then searching below $t = \langle E, 1\rangle$ of the active path is guaranteed not to reduce $ub(B)$ and therefore, the subtree rooted at $\langle E, 1\rangle$ can be pruned.

PROPOSITION **2 (pruning rule)** *Given the active path $\mathcal{AP}(t)$ of a current $\mathcal{PST}$, for any node n on $\mathcal{AP}(t)$, if $f_h(n) \geq ub(n)$ then pruning the subtree below t is safe.*

A depth-first *AND/OR Branch-and-Bound* (AOBB) algorithm that implements this pruning rule is described in Figure 3. A list called OPEN simulates the recursion stack. The list PATH maintains the current assignment (i.e. the active path). $Parent(n)$ refers to the predecessor of n in PATH, which is also the parent in the AND/OR tree, $succ$ denotes the set of successors of a node in the AND/OR tree and $ch_T(X_i)$ denotes the children of variable X_i in T. Procedure LB(n) computes the static heuristic estimate $h(n)$ of $v(n)$.

Step (3) is where the search goes forward and expands alternating levels of OR and AND nodes. Upon the expansion of n, the algorithm successively updates the *lower bound function* $f_h(m)$ for every ancestor m of n along the active path, and discontinues search below n if, for some m, $f_h(m) \geq ub(m)$.

Step (4) is where the value functions are propagated backward. This is triggered when a node has an empty set of successors and it typically happens when the node's descendants are all evaluated or when it is a dead-end. Clearly,

THEOREM **2** *AOBB is sound and complete for COP.*

ALGORITHM: AOBB($\mathcal{P}$, T)
Input: A COP $\mathcal{P} = (\mathcal{X}, \mathcal{D}, \mathcal{F}, +, min)$, pseudo-tree T, root X_0.
Output: Minimal cost solution to $\mathcal{P}$.
(1) Initialize OPEN by adding OR node X_0 to it; PATH $\leftarrow \phi$;
(2) **if** (OPEN == ϕ)
return $v(X_0)$;
Remove the first node n in OPEN; Add n to PATH;
(3) Try to prune the subtree below n:
foreach $m \in PATH$, where m is an ancestor of n
if ($f_h(m) \geq ub(m)$)
$v(n) \leftarrow \infty$; (dead-end)
goto step (4);
Expand n generating all its successors as follows:
$succ(n) \leftarrow \phi$;
if (n is OR node, denote $n = X_i$)
$v(n) \leftarrow \infty$;
foreach value $a \in D_i$
$h(\langle X_i, a\rangle) \leftarrow$ LB(X_i, a);
$succ(n) \leftarrow succ(n) \cup \{\langle X_i, a\rangle\}$;
else (n is AND node, denote $n = \langle X_i, a\rangle$)
$A \leftarrow \{c_j \mid (X_i \in var(c_j)) \wedge (var(c_j) \subseteq$ PATH $)\}$;
$v(n) \leftarrow 0$; $l(X_i, \langle X_i, a\rangle) \leftarrow \sum_A c_j$;
foreach variable $Y \in ch_T(X_i)$
$h(Y) \leftarrow$ LB(Y);
$succ(n) \leftarrow \{Y\}$;
Add $succ(n)$ on top of OPEN;
(4) **while** $succ(n) == \phi$
if (n is OR node)
$v(Parent(n)) \leftarrow v(Parent(n)) + v(n)$;
else (n is AND node)
$v(n) \leftarrow v(n) + l(X_i, \langle X_i, a\rangle)$;
$v(Parent(n)) \leftarrow min(v(Parent(n)), v(n))$;
$succ(Parent(n)) \leftarrow succ(Parent(n)) - \{n\}$;
PATH $\leftarrow$ PATH – $\{n\}$;
$n \leftarrow Last$(PATH);
(5) **goto** step (2);

Figure 3: AND/OR Branch-and-Bound search (AOBB).

While the time complexity of algorithm AOBB is bounded by $O(n \cdot exp(m))$, the size of the AND/OR search space, the pruning rule is designed to yield a far better complexity.

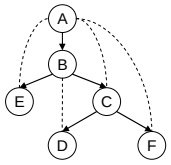
5 Specific Lower Bound Heuristics

In this section we describe briefly two general schemes for generating static heuristic estimates $h(n)$, based on the Mini-Bucket approximation. These schemes are parameterized by the Mini-Bucket i-bound, thus allowing for a controllable trade-off between heuristic strength and its overhead. We also mention a third scheme which is based on the notion of *directional arc-consistency* and is specific to the WCSP model.

5.1 The Mini-Bucket Heuristics

Mini-Bucket Elimination (MBE) [Dechter and Rish, 2003] is an approximation algorithm designed to avoid the high time and space complexity of *Bucket Elimination* (BE) [Dechter, 1999], by partitioning large buckets into smaller subsets, called *mini buckets*, each containing at most i (called i-bound) distinct variables. The mini-buckets are then processed separately. The algorithm outputs not only a bound on the optimal solution cost, but also the collection of augmented buckets, which form the basis for the heuristics generated. The complexity is time and space $O(exp(i))$.

Static Mini-Bucket Heuristics In the past, [Kask and Dechter, 2001] showed that the intermediate functions generated by the Mini-Bucket algorithm MBE(i) can be used to compute a heuristic function, that underestimates the minimal extension of the current assignment in a regular OR search



(a)

B(F): [f(F,A)], [f(F,C)]
B(D): [f(D,B)], [f(D,C)]
B(C): [f(C,A)], [f(C,B) || λ^D(C), λ^F(C)]
B(E): [f(E,B)], [f(E,A)]
B(B): [f(B,A) || λ^E(B), λ^C(B), λ^E(B)]
B(A): [|| λ^E(A), λ^F(A), λ^C(A), λ^B(A)]
(b)

Figure 4: Schematic execution of MBE(2).

tree. In this paper we extend the idea to AND/OR search spaces as well. For that, assume that a COP instance $\mathcal{P}$ with pseudo-tree T is being solved by AOBB search, where the active path ends with some OR node X_j. Consider also the *augmented* bucket structure $\{B(X_1), ..., B(X_n)\}$ of $\mathcal{P}$, constructed along the ordering resulted from a DFS traversal of T. For each possible value assignment $X_j = x_j$, the *static mini-bucket heuristic estimate* $h(x_j)$ of the minimal cost solution rooted at X_j can be computed as the sum of the original functions in bucket $B(X_j)$ and the intermediate functions λ^k that were generated in buckets $B(X_k)$, where X_k is a descendant of X_j in T (more details in [Kask and Dechter, 2001]).

Dynamic Mini-Bucket Heuristics This idea can be pushed one step further. Rather than pre-compiling the mini-bucket heuristic information, it is possible to generate it dynamically, during search. Therefore, the *dynamic mini-bucket heuristic* computes a lower bound by the Mini-Bucket algorithm MBE(i), at each node n in the search space, restricted to the subproblem rooted at n and subject to the current partial instantiation. Specifically, $h(x_j)$ is calculated as the sum of the original and λ^k functions residing in bucket $B(X_j)$, where λ^k's are computed in buckets $B(X_k)$ of X_j's descendants in T, conditioned on the current assignment of the active path.

Example 3 *Figure 4(b) shows the augmented bucket structure generated by MBE(i=2) for the binary COP instance displayed in Figure 4(a), along the ordering* (A, B, E, C, D, F)*; square brackets denote the choice of partitioning. Assume that during search, the active path of the current partial solution subtree is* $(A = a, B = b)$ *and the tip node is the OR node* C*. The static mini-bucket heuristic estimate* $h(C = c) = f(c, a) + f(c, b) + \lambda^F(a) + \lambda^F(c) + \lambda^D(c) + \lambda^D(b)$*. The dynamic mini-bucket heuristic estimate* $h(C = c)$*, involves the same* λ *functions generated in buckets* $B(F)$ *and* $B(D)$*, only that the* λ*'s are now computed dynamically, conditioned on the current partial assignment* $(A = a, B = b)$.

5.2 Directional Arc-Consistency Heuristics

We also adapted for the AND/OR search space two other successful heuristics generators, *reversible DAC counts* (RDAC) [Meseguer *et al.*, 1999] and *maintaining full DAC* (MFDAC) [Larrosa and Schiex, 2003], which proved powerful for solving binary Weighted CSPs (details omitted for space reasons).

6 Experiments

In this section we evaluate empirically the performance of our new AND/OR Branch-and-Bound approach on two classes of

Network (n,d,c,t) [w*,h] connectivity	s-AOMB s-BBMB d-AOMB d-BBMB i=2		s-AOMB s-BBMB d-AOMB d-BBMB i=4		s-AOMB s-BBMB d-AOMB d-BBMB i=6		s-AOMB s-BBMB d-AOMB d-BBMB i=8		AORDAC BBRDAC AOMFDAC BBMFDAC	
	time	nodes	time	nodes	time	nodes	time	nodes	time	nodes
(20,5,100,0.7)	-	2.4M	115.57	2.5M	15.49	408K	**6.91**	126K	21.70	441K
[12,15]	-	6.3M	179.34	7.6M	127.77	6.5M	45.76	2.2M	24.74	1.3M
medium	74.43	90K	51.19	6.9K	104.08	751	169.30	101	9.99	20K
	124.45	523K	80.79	34K	140.10	3.3K	176.33	537	8.75	21.3K
(30,5,90,0.7)	-	2.8M	105.77	2.2M	9.84	262K	**2.71**	28K	78.50	1.3M
[11,16]	-	6M	180.00	7.5M	68.90	3.3M	5.64	230K	78.24	4.2M
low	72.94	82K	31.85	4.3K	63.07	548	94.95	111	10.72	22.2K
	104.15	348K	69.49	22K	90.70	1.7K	123.42	265	8.79	31.4K
(50,5,80,0.7)	67.53	1.4M	1.80	57K	**0.12**	2.6K	0.62	356	28.90	691K
[8,16]	-	5M	145.39	4.3M	24.47	804K	1.58	36K	155.58	3.9M
sparse	7.91	18.6K	1.17	430	0.95	87	2.31	60	1.48	8.5K
	63.50	295K	1.83	1K	0.94	112	2.34	69	1.49	14K

Table 1: Results on random binary WCSP instances.

optimization problems: Weighted CSP (WCSP) and the Most Probable Explanation (MPE) problem in belief networks[2].

Weighted CSP [Bistarelli *et al.*, 1997; Larrosa and Schiex, 2003] extends the classic CSP formalism with so-called *soft constraints* which assign positive integer costs to forbidden tuples (allowed tuples have cost 0). The goal is to find a complete assignment with minimum aggregated cost. The model has numerous applications in domains such as *resource allocation*, *combinatorial auctions* or *bioinformatics*.

Belief Networks [Pearl, 1988] provide a formalism for reasoning under conditions of uncertainty. A belief network represents a joint probability distribution over the variables of interest. A function of the graphical model encodes *conditional probability distribution* of a variable given its parents in the graph (also viewed as a cost function were each tuple has associated a real cost between 0 and 1). The MPE problem is the task of finding a complete assignment with maximum probability that is consistent with the evidence. It appears in applications such as *speech recognition* or *medical diagnosis*.

The *pseudo-tree* was created as suggested in [Bayardo and Miranker, 1995], by a DFS traversal of the induced graph. The latter was computed using the *min-fill* heuristic. All competing algorithms were restricted to a static variable ordering resulted from a DFS traversal of the pseudo-tree. We report the average effort, as CPU time (in seconds) and number of visited nodes (AND nodes only for the AND/OR algorithms), required for proving optimality of the solution. For all test instances we record the number of variables (n), domain size (d), number of functions (c), induced width (w*) and height of the pseudo-tree (h). A "-" indicates that a time limit was exceeded by the respective algorithm. The best results are highlighted.

6.1 Weighted CSP

For this domain we experimented with random binary WCSP problems as well as real-world benchmarks. We consider four classes of AND/OR Branch-and-Bound (AOBB) algorithms, each using a specific heuristics generator, as follows. Classes s-AOMB/d-AOMB are guided by static/dynamic mini-bucket heuristics, AORDAC uses RDAC based heuristics, and AOMFDAC maintains full DAC. For comparison, we include results obtained with the classic OR version of each class of algorithms, denoted here by s-BBMB, d-BBMB, BBRDAC and BBMFDAC, respectively.

[2]All our experiments were done on a 2.4GHz Pentium IV with 1GB of RAM, running Windows XP

Network	(n,d,c,w*,h)	BBMFDAC time (sec)	BBMFDAC nodes	AOMFDAC time (sec)	AOMFDAC nodes
CELAR6-SUB0	(16,44,57,7,10)	2.78	1,871	**1.98**	435
CELAR6-SUB1	(14,44,75,9,11)	2420.93	364,986	**981.98**	180,784
CELAR6-SUB2	(16,44,89,10,13)	8801.12	19,544,182	**1138.87**	175,377
CELAR6-SUB3	(18,44,106,10,13)	38889.20	91,168,896	**4028.59**	846,986
CELAR6-SUB4	(22,44,131,11,16)	84478.40	6,955,039	**47115.40**	4,643,229

Table 2: Results on CELAR6 subinstances.

Random Binary Networks

Our random binary WCSP class is characterized by a five parameter model $\langle n, d, c, t, w \rangle$ [Larrosa and Schiex, 2003], where n is the number of variables, d the domain size, c the number of constraints, and t the constraint *tightness* defined as the ratio of forbidden tuples. The costs of inconsistent tuples are uniformly randomly distributed between 1 and w.

Table 1 shows results for experiments with three problem classes containing instances with medium, low and very low connectivity. We chose a maximum penalty cost w of 10 and set the constraint tightness to 70% in order to obtain over-constrained problems. For each problem class we generated 20 instances and the time limit was set to 180 seconds. The columns are indexed by the i-bound of the mini-bucket heuristics. When comparing AND/OR versus OR algorithms we notice a considerable improvement in terms of CPU time and number of nodes visited, especially for problems with low and very low connectivity. This observation verifies the theory because a relatively sparse problem is likely to produce a shallow pseudo-tree, which in turn enhances the performance of the AND/OR algorithms. In terms of the quality of the heuristics, we also observe that the static mini-buckets with a relatively large i-bound represent the best choice. However, if large i-bounds are not possible, dynamic mini-buckets with small i-bounds are preferred, especially for sparse problems. For medium and low connected problems, MFDAC proves to be cost effective with respect to the other heuristics generators.

Radio Link Frequency Assignment Problem (RLFAP)

RLFAP is a communication problem where the goal is to assign frequencies to a set of radio links in such a way that all links may operate together without noticeable interferences [Cabon *et al.*, 1999]. It can be naturally casted as a binary WCSP where each forbidden tuple has an associated penalty cost. Table 2 compares algorithms BBMFDAC and AOMFDAC for solving 5 publicly available RLFAP subinstances called $\texttt{CELAR6-SUB}_i$ $(i = 0, ..., 4)$. We can see that the AND/OR approach is beneficial for this domain as well. In $\texttt{CELAR6-SUB}_4$, the hardest instance, AOMFDAC causes a CPU speed up of 1.8, whereas in $\texttt{CELAR6-SUB}_3$ the speed up is as much as 9.6. We also compared AOMFDAC against BTD, a recent algorithm introduced in [Jegou and Terrioux, 2004]. BTD solves the MAX-CSP version of $\texttt{CELAR6-SUB}_4$ (i.e. 0/1 penalty costs) in about 123,000 sec., whereas AOMFDAC proves optimality in only 2,574 sec. The performance of the mini-bucket based algorithms was quite poor on this domain, due to the very low quality of the heuristic estimates resulted from approximating subproblems with very large domains (up to 44 values).

Network (n,d,w*,h)	s-AOMB s-BBMB d-AOMB d-BBMB i=2		s-AOMB s-BBMB d-AOMB d-BBMB i=3		s-AOMB s-BBMB d-AOMB d-BBMB i=4		s-AOMB s-BBMB d-AOMB d-BBMB i=5	
	time	nodes	time	nodes	time	nodes	time	nodes
Mildew	4.58	55K	0.50	5,465	**0.28**	35	0.66	35
(35,100,4,15)	-	26M	233.86	6.9M	0.47	4,970	0.81	4,940
	86.38	15K	34.45	1,424	1.69	35	3.02	35
	162.61	83K	41.92	5,113	1.78	363	3.13	363
Barley	-	8.5M	-	7.6M	46.22	807K	**0.56**	9.6K
(48,67,7,17)	-	16M	-	18M	-	17M	-	14M
	-	79K	135.97	23K	12.55	667	45.95	567
	-	2.2M	-	1K	346.08	76K	-	86K
Munin1	57.36	1.2M	12.08	260K	7.20	172K	**1.66**	43K
(189,21,11,24)	-	8.5M	-	9.2M	-	9.9M	-	8.3K
	66.56	185K	12.47	8.1K	10.30	1.6K	11.99	523
	-	405K	-	430K	-	235K	14.63	917
Munin2	-	5.6M	-	6.7M	116.19	1.8M	**1.64**	21K
(1003,21,7,35)	-	1.7M	-	2.7M	-	430K	-	428K
	-	3.2M	-	1.2M	524.54	299K	39.22	3.8K
	-	33K	-	131K	-	101K	-	20K
Munin3	-	5.9M	-	4.9M	1.31	17K	**0.45**	6.2K
(1044,21,7,25)	-	1.4M	-	1.2M	-	316K	-	1.5M
	-	2.4M	68.64	58K	3.59	5.9K	2.84	3.8K
	-	33K	-	125K	-	52K	-	31K
Pigs	-	15M	**0.02**	441	**0.02**	441	**0.02**	441
(441,3,10,27)	-	2.8M	0.63	4.2K	0.63	4K	0.61	4K
	-	6.5M	0.08	441	0.08	441	0.11	441
		2.2M	1.03	614	1.08	614	1.11	614

Table 3: Results on Bayesian Network Repository.

6.2 Belief Networks

For the MPE domain we also experimented with random networks and real-world benchmarks, but we only report on the latter due to space limitations. We compare the algorithms using the mini-bucket based heuristics generators, namely s-AOMB, d-AOMB, s-BBMB and d-BBMB. Notice that s-BBMB is currently one of the best performing complete algorithms for this domain [Kask and Dechter, 2001]

Table 3 summarizes the results for experiments on 6 real-world belief networks from the Bayesian Network Repository[3]. The time limit was set to 600 seconds. We observe again a considerable improvement of the new AND/OR algorithms over the corresponding OR ones. If we look, for example, at the Mildew instance, s-AOMB(3) causes a CPU speedup of 468 over s-BBMB(3). In conclusion, d-AOMB is superior for relatively small i-bounds (e.g. Barley, Munin3), whereas s-AOMB dominates for larger i-bounds.

7 Conclusion

The paper investigates the impact of the AND/OR search space for graphical models on optimization tasks. We introduce a general AND/OR Branch-and-Bound algorithm and specialize it with several schemes for generating heuristic estimates that can guide the search. We focus on two common optimization problems, WCSP and Bayesian MPE, and show empirically that the new AND/OR algorithms improve dramatically over traditional OR ones on a variety of benchmarks including random and real-world problems.

Our approach leaves room for future improvements. For instance, it can be modified to traverse an AND/OR graph, rather than a tree, via caching. We should consider the effect of dynamic variable ordering. Also, we used a rather simple scheme of generating pseudo-tree arrangements, probably having non-optimal height.

[3]http://www.cs.huji.ac.il/labs/compbio/Repository

Related Work: AOBB is related to the Branch-and-Bound method proposed by [Kanal and Kumar, 1988] for acyclic AND/OR graphs and game trees. More recently, [Larrosa *et al.*, 2002] extended pseudo-tree search [Freuder and Quinn, 1985] to optimization tasks in order to boost the Russian Doll search for solving Weighted CSPs. The optimization method developed in [Jegou and Terrioux, 2004] can also be interpreted as an AND/OR search graph algorithm, however it is not a linear space algorithm.

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