

Parallel Recursive Best-First AND/OR Search for Exact MAP Inference in Graphical Models

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Abstract

The paper presents and evaluates the power of parallel search for exact MAP inference in graphical models. We introduce a new parallel shared-memory recursive best-first AND/OR search algorithm, called SPRBFAOO, that explores the search space in a best-first manner while operating with restricted memory. Our experiments show that SPRBFAOO is often superior to the current state-of-the-art sequential AND/OR search approaches, leading to considerable speed-ups (up to 7-fold with 12 threads), especially on hard problem instances.

1 Paper Body

Graphical models provide a powerful framework for reasoning with probabilistic information. These models use graphs to capture conditional independencies between variables, allowing a concise knowledge representation and efficient graph-based query processing algorithms. Combinatorial maximization, or maximum a posteriori (MAP) tasks arise in many applications and often can be efficiently solved by search schemes, especially in the context of AND/OR search spaces that are sensitive to the underlying problem structure [1]. Recursive best-first AND/OR search (RBFAOO) is a recent yet very powerful scheme for exact MAP inference that was shown to outperform current state-of-the-art depth-first and best-first methods by several orders of magnitude on a variety of benchmarks [2]. RBFAOO explores the context minimal AND/OR search graph associated with a graphical model in a best-first manner (even with nonmonotonic heuristics) while running within restricted memory. RBFAOO extends Recursive BestFirst Search (RBFS) [3] to graphical models and thus uses a threshold controlling technique to drive the search in a depth-first like manner while using the available memory for caching. Up to now, search-based MAP solvers were developed primarily as sequential search algorithms. However, parallel, multi-core processing can be a powerful approach to boosting the performance of a problem solver.

Now that multi-core computing systems are ubiquitous, one way to extract substantial speed-ups from the hardware is to resort to parallel processing. Parallel search has been successfully employed in a variety of AI areas, including planning [4], satisfiability [5], and game playing [6, 7]. However, little research has been devoted to solving graphical models in parallel. The only parallel search scheme for MAP inference in graphical models that we are aware of is the distributed AND/OR Branch and Bound algorithm (daoopt) [8]. This assumes however a large and distributed computational grid environment with hundreds of independent and loosely connected computing systems, without access to a shared memory space for caching and reusing partial results. Contribution In this paper, we take a radically different approach and explore the potential of parallel search for MAP tasks in a shared-memory environment which, to our knowledge, has not been attempted before. We introduce SPRBFAOO, a new parallelization of RBFAOO in sharedmemory environments. SPRBFAOO maintains a single cache table shared among the threads. In this way, each thread can effectively reuse the search effort performed by others. Since all threads start from the root of the search graph using the same search strategy, an effective load balancing is 1

- (a) Primal graph
- (b) Pseudo tree
- (c) Context minimal AND/OR search graph

Figure 1: A simple graphical model and its associated AND/OR search graph, obtained without using sophisticated schemes, as done in previous work [8]. An extensive empirical evaluation shows that our new parallel recursive best-first AND/OR search scheme improves considerably over current state-of-the-art sequential AND/OR search approaches, in many cases leading to considerable speed-ups (up to 7-fold using 12 threads) especially on hard problem instances.

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Background

Graphical models (e.g., Bayesian Networks [9] or Markov Random Fields [10]) capture the factorization structure of a distribution over a set of variables. A graphical model is a tuple $M = \langle X, D, F \rangle$, where $X = \{X_i : i \in V\}$ is a set of variables indexed by set V and $D = \{D_i : i \in V\}$ is the set of their finite domains of values. $F = \{f : \varphi \rightarrow \mathbb{R}^+\}$ is a set of discrete positive realvalued local functions defined on subsets of variables, where $\varphi \subseteq V$ is a set of variable subsets. We use $\varphi \subseteq V$ and $X_\varphi \subseteq X$ to indicate the scope of function f , i.e., $X_\varphi = \text{var}(\varphi) = \{X_i : i \in \varphi\}$. The function scopes yield a primal graph whose vertices are the variables and whose edges connect any two variables that appear in the scope of the same function. The graphical model M defines a factorized probability distribution on X , as follows: $P(X) = \frac{1}{Z} \prod_{f \in F} f(X_\varphi)$ where the partition function, Z , normalizes the probability. An important inference task which appears in many real world applications is maximum a posteriori (MAP, sometimes called maximum probable explanation or MPE). MAP/MPE finds a complete assignment to the variables Q that has the highest probability (i.e., a mode of the joint probability), namely: $x^* = \arg\max_x \prod_{f \in F} f(x_\varphi)$. The task is NP-hard to solve in general [9]. In this paper we focus on solving

MAP as a minimization problem by taking P the negative logarithm of the local functions to avoid numerical issues, namely: $x^* = \operatorname{argmin}_x \sum_i F_i(x)$. Significant improvements for MAP inference have been achieved by using AND/OR search spaces, which often capture problem structure far better than standard OR search methods [11]. A pseudo tree of the primal graph captures the problem decomposition and is used to define the search space. A pseudo tree of an undirected graph $G = (V, E)$ is a directed rooted tree $T = (V, E_0)$, such that every arc of G not included in E_0 is a back-arc in T , namely it connects a node in T to an ancestor in T . The arcs in E_0 may not all be included in E . Given a graphical model $M = \langle X, D, F \rangle$ with a primal graph G and a pseudo tree T of G , the AND/OR search tree ST has alternating levels of OR nodes corresponding to the variables and AND nodes corresponding to the values of the OR parent's variable, with edges weighted according to F . We denote the weight on the edge from OR node n to AND node m by $w(n, m)$. Identical subproblems, identified by their context (the partial instantiation that separates the sub-problem from the rest of the problem graph), can be merged, yielding an AND/OR search graph [11]. Merging all context-mergeable nodes yields the context minimal AND/OR search graph, denoted by CT . The size of CT is exponential in the induced width of G along a depth-first traversal of T [11]. A solution tree T of CT is a subtree such that: (1) it contains the root node of CT ; (2) if an internal AND node n is in T then all its children are in T ; (3) if an internal OR node n is in T then exactly one of its children is in T ; (4) every tip node in T (i.e., nodes with no children) is a terminal node. The cost of a solution tree is the sum of the weights associated with its edges. 2

Each node n in CT is associated with a value $v(n)$ capturing the optimal solution cost of the conditioned sub-problem rooted at n . It was shown that $v(n)$ can be computed recursively based on the values of n 's children: OR nodes by minimization, AND nodes by summation (see also [11]). Example 1. Figure 1(a) shows the primal graph of a simple graphical model with 5 variables and 7 binary functions. Figure 1(c) displays the context minimal AND/OR search graph based on the pseudo tree from Figure 1(b) (the contexts are shown next to the pseudo tree nodes). A solution tree corresponding to the assignment $(A = 0, B = 1, C = 1, D = 0, E = 0)$ is shown in red. Current state-of-the-art sequential search methods for exact MAP inference perform either depthfirst or best-first search. Prominent methods studied and evaluated extensively are the AND/OR Branch and Bound (AOBB) [1] and Best-First AND/OR Search (AOBF) [12]. More recently, Recursive Best-First AND/OR Search (RBFAOO) [2] has emerged as the best performing algorithm for exact MAP inference. RBFAOO belongs to the class of RBFS algorithms and employs a local threshold controlling mechanism to explore the AND/OR search graph in a depth-first like manner [3, 13]. RBFAOO maintains at each node n a lower-bound $q(n)$ (called q -value) on $v(n)$. During search, RBFAOO improves and caches in a fixed size table $q(n)$ which is calculated by propagating back the q -values of n 's children. RBFAOO stops when $q(r) = v(r)$ at the root r or it proves that there is no solution, namely $q(r) = v(r) = \infty$.

Our Parallel Algorithm

Algorithm 1 SPRBFAO for all i from 1 to nr CPU cores do $root.th \ ? \ ? \ ?$
 $; root.thub \ ? \ ? \ launch \ tRBFS(root)$ on a separate thread wait for threads to
 finish their work return optimal cost (e.g., as $root$'s q -value in the cache)

We now describe SPRBFAO, a parallelization of RBFAO in shared-memory environments. SPRBFAO's threads start from the root and run in parallel, as shown in Algorithm 1. Threads share one cache table, allowing them to reuse the results of each other. An entry in the cache table, corresponding to a node n , is a tuple with 6 fields: a q -value $q(n)$, being a lower bound on the optimal cost of node n ; $n.solved$, a flag indicating whether n is solved optimally; a virtual q -value $vq(n)$, defined later in this section; a best known solution cost $bs(n)$ for node n ; the number of threads currently working on n ; and a lock. When accessing a cache entry, threads lock it temporarily for other threads. The method $Ctxt(n)$ identifies the context of n , which is further used to access the corresponding cache entry. Besides the cache, shared among threads, each thread will use two threshold values, $n.th$ and $n.thub$, for each node n . These are separated from one thread to another. Algorithm 2 shows the procedure invoked on each thread. When a thread examines a node n , it first increments in the cache the number of threads working on node n (line 1). Then it increases $vq(n)$ by an increment $?$, and stores the new value in the cache (line 2). The virtual q -value $vq(n)$ is initially set to $q(n)$. As more threads work on solving n , $vq(n)$ grows due to the repeated increases by $?$. In effect, $vq(n)$ reflects both the estimated cost of node n (through its $q(n)$ component) and the number of threads working on n . By computing $vq(n)$ this way, our goal is to dynamically control the degree to which threads overlap when exploring the search space. When a given area of the search space is more promising than others, more than one thread are encouraged to work together within that area. On the other hand, when several areas are roughly equally promising, threads should diverge and work on different areas. Indeed, in Algorithm 2, the tests on lines 13 and 23 prevent a thread from working on a node n if $n.th \geq vq(n)$. (Other conditions in these tests are discussed later.) A large $vq(n)$, which increases the likelihood that $n.th \geq vq(n)$, may reflect a less promising node (i.e., large q -value), or many threads working on n , or both. Thus, our strategy is an automated and dynamic way of tuning the number of threads working on solving a node n as a function of how promising that node is. We call this the thread coordination mechanism. Lines 4-7 address the case of nodes with no children, which are either terminal nodes or deadends. In both cases, method $Evaluate$ sets the solved flag to true. The q -value q is set to 0 for terminal 3

Algorithm 2 Method $tRBFS$. Handling locks skipped for clarity. Require: node n 1: $IncrementNrThreadsInCache(Ctxt(n))$ 2: $IncreaseVQInCache(Ctxt(n), ?)$ 3: if n has no children then 4: $(q, solved) \leftarrow Evaluate(n)$ 5: $SaveInCache(Ctxt(n), q, solved, q, q)$ 6: $DecrementNrThreadsInCache(Ctxt(n))$ 7: return 8: $GenerateChildren(n)$ 9: if n is an OR node then 10: loop 11: $(cbest, vq, vq2, q, bs) \leftarrow BestChild(n)$ 12: $n.thub \leftarrow \min(n.thub, bs)$ 13: if $n.th \geq vq$? q ? $n.thub$? $n.solved$ then 14: break 15: $cbest.th \leftarrow \min(n.th, vq2 + ?)w(n, cbest)$ 16: $cbest.thub \leftarrow n.thub$? $w(n, cbest)$ 17: $tRBSF(cbest)$

18: [continued from previous column] 19: if n is an AND node then 20: loop
21: (q , vq , bs) ? Sum(n) 22: $n.thub$? $\min(n.thub, bs)$ 23: if $n.thub \leq vq$? q
? $n.thub \leq n.solved$ then 24: break 25: ($cbest$, $qcbest$, $vqcbest$) ? Unsolved-
Child(n) 26: $cbest.th$? $n.th$? (vq ? $vqcbest$) 27: $cbest.thub$? $n.thub$?
(q ? $qcbest$) 28: $tRBSF(cbest)$ 29: if $n.solved$? $NrThreadsCache(Ctxt(n))$
 $= 1$ then 30: vq ? q 31: Decrement $NrThreadsInCache(Ctxt(n))$ 32: SaveIn-
Cache($Ctxt(n)$, q , $n.solved$, vq , bs)

nodes and to ? otherwise. Method SaveInCache takes as argument the context of the node, and four values to be stored in order in these fields of the corresponding cache entry: q , solved, vq and bs . Lines 10?17 and 20?28 show respectively the cases when the current node n is an OR node or an AND node. Both these follow a similar high-level sequence of steps: ? Update vq , q , and bs for n , from the children's values (lines 11, 21). Also update $n.thub$ (lines 12, 22), an upper bound for the best solution cost known for n so far. Methods BestChild and Sum are shown in Algorithm 3. In these, child node information is either retrieved from the cache, if available, or initialized with an admissible heuristic function h . ? Perform the backtracking test (lines 13?14 and 23?24). The thread backtracks to n 's parent if at least one of the following conditions hold: $th(n) \leq vq(n)$, discussed earlier; $q(n) \leq n.thub$ i.e., a solution containing n cannot possibly beat the best known solution (we call this the suboptimality test); or the node is solved. The solved flag is true iff the node cost has been proven to be optimal, or the node was proven not to have any solution. ? Otherwise, select a successor $cbest$ to continue with (lines 11, 25). At OR nodes n , $cbest$ is the child with the smallest vq among all children not solved yet (see method BestChild). At AND nodes, any unsolved child can be chosen. Then, update the thresholds of $cbest$ (lines 15?16 and 26?27), and recursively process $cbest$ (lines 17, 28). The threshold $n.th$ is updated in a similar way to RBFAOO, including the overestimation parameter ? (see [2]). However, there are two key differences. First, we use vq instead of q , to obtain the thread coordination mechanism presented earlier. Secondly, we use two thresholds, th and $thub$, instead of just th , with $thub$ being used to implement the suboptimality test $q(n) \leq n.thub$. When a thread backtracks to n 's parent, if either n 's solved flag is set, or no other thread currently examines n , the thread sets $vq(n)$ to $q(n)$ (lines 29?30 in Algorithm 2). In this way, SPRBFAOO reduces the frequency of the scenarios where n is considered to be less promising. Finally, the thread decrements in the cache the number of threads working on n (line 31), and saves in the cache the recalculated $vq(n)$, $q(n)$, $bs(n)$, and the solved flag (line 32). Theorem 3.1. With an admissible heuristic in use, SPRBFAOO returns optimal solutions. Proof sketch. SPRBFAOO's $bs(r)$ at the root r is computed from a solution tree, therefore, $bs(r) \leq v(r)$. Additionally, SPRBFAOO determines solution optimality by using not $vq(n)$ but $q(n)$ saved in the cache table. By an induction-based discussion similar to Theorem 3.1 in [2], $q(n) \leq v(n)$ holds for any $q(n)$ saved in the cache table with admissible h , which indicates $q(r) \leq v(r)$. When SPRBFAOO returns a solution, $bs(r) = q(r)$, therefore, $bs(r) = q(r) = v(r)$. We conjecture that SPRBFAOO is also complete, and leave a more in-depth analysis as future work. 4

Algorithm 3 Methods BestChild (left) and Sum (right) Require: node n
 Require: node n 1: n.solved ? ? (? stands for false); 1: n.solved ? ; (stands for true) 2: initialize vq, vq2, q, bs to ? 2: initialize vq, q, bs to 0 3: for all ci child of n do 3: for all ci child of n do 4: if Ctxt(ci) in cache then 4: if Ctxt(ci) in cache then 5: (qci, sci, vqci, bsci) ? FromCache(Ctxt(ci)) 5: (qci, sci, vqci, bsci) ? FromCache(Ctxt(ci)) 6: else 6: else 7: (qci, sci, vqci, bsci) ? (h(ci), ?, h(ci), ?) 7: (qci, sci, vqci, bsci) ? (h(ci), ?, h(ci), ?) 8: qci ? w(n, ci) + qci 8: q ? q + qci 9: vqci ? w(n, ci) + vqci 9: vq ? vq + vqci 10: bs = min(bs, w(n, ci) + bsci) 10: bs ? bs + bsci 11: if (qci < q) ? (qci = q ? ?n.solved) then 11: n.solved ? n.solved ? sci 12: n.solved ? sci ; q ? qci 12: return (q, vq, bs) 13: if vqci < vq ? ?sci then 14: vq2 ? vq; vq ? vqci ; cbest ? ci 15: else if vqci < vq2 ? ?sci then 16: vq2 ? vqci 17: return (cbest, vq, vq2, q, bs)

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Experiments

We evaluate empirically our parallel SPRBFAOO and compare it against sequential RBFAOO and AOBB. We also considered parallel shared-memory AOBB, denote by SPAOBB, which uses a master thread to explore centrally the AND/OR search graph up to a certain depth and solves the remaining conditioned sub-problems in parallel using a set of worker threads. The cache table is shared among the workers so that some workers may reuse partial search results recorded by others. In our implementation, the search space explored by the master corresponds to the first m variables in the pseudo tree. The performance of SPAOBB was very poor across all benchmarks due to noticeably large search overhead as well as poor load balancing, and therefore its results are omitted hereafter. All competing algorithms (SPRBFAOO, RBFAOO and AOBB) use the pre-compiled mini-bucket heuristic [1] for guiding the search. The heuristic is controlled by a parameter called i -bound which allows a trade-off between accuracy and time/space requirements. Higher values of i yield a more accurate heuristic but take more time and space to compute. The search algorithms were also restricted to a static variable ordering obtained as a depth-first traversal of a min-fill pseudo tree [1]. Our benchmark problems include three sets of instances from genetic linkage analysis (denoted pedigree) [14], grid networks and protein side-chain interaction networks (denoted protein) [15]. In total, we evaluated 21 pedigrees, 32 grids and 240 protein networks. The algorithms were implemented in C++ (64-bit) and the experiments were run on a 2.6GHz 12-core processor with 80GB of RAM. Following [2], RBFAOO ran with a 10-20GB cache table (134,217,728 entries) and overestimation parameter $\epsilon = 1$. However, SPRBFAOO allocated only 95,869,805 entries with the same amount of memory, due to extra information such as virtual q -values. We set $\epsilon = 0.01$ throughout the experiments (except those where we vary ϵ). The time limit was set to 2 hours. We also record typical ranges of problem specific parameters shown in Table 1 such as the number of variables (n), maximum domain size (k), induced width ($w?$), and depth of the pseudo tree (h). Table 1: Ranges (min-max) of the benchmark problems parameters. benchmark grid pedigree protein

n 144 ? 676 334 ? 1289 26 ? 177

k 2 3?7 81

w? 15 ? 36 15 ? 33 6 ? 16

Table 2: Number of unsolved problem instances (1 vs 12 cores).

h 48 ? 136 51 ? 140 15 ? 43

method RBFAOO SPRBFAOO

grid i = 6 i = 14 9 5 7 5

pedigree i = 6 i = 14 8 6 7 3

protein i = 2 i=4 41 16 32 9

The primary performance measures reported are the run time and node expansions during search. When the run time of a solver is discussed, the total CPU time reported in seconds is one metric to show overall performance. The total CPU time consists of the heuristic compilation time and search 1

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

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Table 3: Total CPU time (sec) and nodes on grid and pedigree instances. Time limit 2 hours. instance (n, k, w? , h) 75-22-5 (484,2,30,107)

75-24-5 (576,2,32,116)

90-30-5 (900,2,42,151)

pedigree7 (1068,4,28,140)

pedigree9 (1119,7,25,123)

pedigree19 (793,5,21,107)

(mbe) AOBB RBFAOO SPRBFAOO (mbe) AOBB RBFAOO SPRBFAOO

(mbe) AOBB RBFAOO SPRBFAOO (mbe) AOBB RBFAOO SPRBFAOO (mbe)

AOBB RBFAOO SPRBFAOO (mbe) AOBB RBFAOO SPRBFAOO

i=8

time (0.06

nodes

time (0.07)

nodes

629 116 (0.08)

133143216 153612683

2018 483 (0.1)

331885596 410230906

2794 (0.2)

2273916962

2959 (0.2)

2309390159

(0.1)

(0.2)

(0.1)

4560 (0.2)

(0.1)

(0.2)

grids : total CPU time, i-bound (i = 6)

SPRBFAOO

SPRBFAOO
 101
 3062954989
 103
 226436502 249562472
 201063828 222896697
 (1.3)
 102
 104
 104
 2721253097
 101
 101
 102
 103
 104
 144092486 18728991 25076772
 229 43 (1.4)
 47015068 59504303
 3783 869 (2.1)
 565053698 665947009
 1239 267 (1.6)
 135387634 151794050
 3021 (10)
 2807834881
 2083
 1914585138
 protein : total CPU time, i-bound (i = 2)
 102
 100 0 10
 104
 101
 pedigree : total CPU time, i-bound (i = 14)
 103
 104
 104
 protein : total CPU time, i-bound (i = 4)
 103
 102
 100 0 10
 102
 RBFAOO
 101
 103
 nodes
 101

SPRBFAOO
 SPRBFAOO
 102
 102
 1642 314 (0.5)
 (0.4)
 103
 RBFAOO
 465384385 511894256
 RBFAOO
 grids : total CPU time, i-bound (i = 14)
 101
 314622599 113597702 129817500
 time (0.7) 884 85 17 (0.8)
 103
 100 0 10
 104
 103
 SPRBFAOO
 1873 353 (0.2)
 i = 14 nodes
 (0.6)
 101
 102
 2792 579 (0.5)
 (0.3)
 RBFAOO
 100 0 10
 665237411 804068930
 103
 101
 i = 12 time (0.2) 2100 638 152 (0.3)
 761867041 334441548 385071090
 pedigree : total CPU time, i-bound (i = 6)
 104
 102
 104
 4182 1012 (0.3)
 i = 10 nodes
 3792
 103
 100 0 10
 time (0.1) 5221 2036 466 (0.1)
 SPRBFAOO
 104
 i=6

```

algorithm
102
101
101
102
RBFAOO
103
104
100 0 10
101
102
103
104
RBFAOO

```

Figure 2: Total CPU time (sec) for RBFAOO vs. SPRBFAOO with smaller (top) and larger (bottom) i-bounds. Time limit 2 hours. $i \in \{6, 14\}$ for grid and pedigree, $i \in \{2, 4\}$ for protein. time. SPRBFAOO does not reduce the heuristic compilation time calculated sequentially. Note that parallelizing the heuristic compilation is an important extension as future work. Parallel versus sequential search Table 3 shows detailed results (as total CPU time in seconds and nodes expanded) for solving grid and pedigree instances using parallel and sequential search. The columns are indexed by the i-bound. For each problem instance, we also record the mini-bucket heuristic pre-compilation time, denoted by (mbe), corresponding to each i-bound. SPRBFAOO ran with 12 threads. We can see that SPRBFAOO improves considerably over RBFAOO across all reported i-bounds. The benefit of parallel search is more clearly observed at smaller i-bounds that correspond to relatively weak heuristics. In this case, the heuristic is less likely to guide the search towards more promising regions of the search space and therefore diversifying the search via multiple parallel threads is key to achieving significant speed-ups. For example, on grid 75-225, SPRBFAOO(6) is almost 6 times faster than RBFAOO(6). Similarly, SPRBFAOO(8) solves the pedigree7 instance while RBFAOO(8) runs out of time. This is important since on very hard problem instances it may only be possible to compute rather weak heuristics given limited resources. Notice 6

```

6
30000
Average speed-up
Total search time (sec)
35000
25000 20000 15000
grids pedigree protein
10000 5000
5 4 3 2
grids pedigree protein
1 0
0

```

0.001
0.01 parameter ?
0.1
0.001
0.01 parameter ?
0.1

Figure 3: Total search time (sec) and average speed-up as a function of parameter i . Time limit 2 hours. $i = 14$ for grid and pedigree, $i = 4$ for protein. also that the pre-processing time (mbe) increases with the i -bound. Table 2 shows the number of unsolved problems in each domain. Note that SPRBFAO solved all instances solved by RBFAO. Figure 2 plots the total CPU time obtained by RBFAO and SPRBFAO using smaller (resp. larger) i -bounds corresponding to relatively weak (resp. strong) heuristics. We selected $i \in \{6, 14\}$ for grid and pedigree, and $i \in \{2, 4\}$ for protein. Specifically, $i = 6$ (grids, pedigrees) and $i = 2$ (proteins) were the smallest i -bounds for which SPRBFAO could solve at least two thirds of instances within the 2 hour time limit, while $i = 14$ (grids, pedigrees) and $i = 4$ (proteins) were the largest possible i -bounds for which we could compile the heuristics without running out of memory on all instances. The data points shown in green correspond to problem instances that were solved only by SPRBFAO. As before, we notice the benefit of parallel search when using relatively weak heuristics. The largest speed-up of 9.59 is obtained on the pdbulk protein instance with $i = 2$. As the i -bound increases and the heuristics become more accurate, the difference between RBFAO(i) and SPRBFAO(i) decreases because both algorithms are guided more effectively towards the subspace containing the optimal solution. In addition, the overhead associated with larger i -bounds, which is calculated sequentially, offsets considerably the speed-up obtained by SPRBFAO(i) over RBFAO(i) (see for example the plot for protein instances with $i = 4$). We also observed that SPRBFAO's speed-up over RBFAO increases sublinearly as more threads are used (we experimented with 3, 6, and 12 threads, respectively). In addition to search overhead, synchronization overhead is another cause for achieving only sublinear speed-ups. The synchronization overhead can be estimated by checking the node expansion rate per thread. For example, in case of SPRBFAO with 12 threads, the node expansion rate per thread slows down to 47 %, 50 %, and 61 % of RBFAO in grid ($i = 6$), pedigree ($i = 6$), and protein ($i = 2$), respectively. This implies that the overhead related to locks is large. Since these numbers with 6 threads are 73 %, 79 %, and 96 %, respectively, the slowdown becomes severer with more threads. We hypothesize that due to the property of the virtual q -value, SPRBFAO's threads tend to follow the same path from the root until search directions are diversified, and frequently access the cache table entries of these internal nodes located on that path, where lock contentions occur non-negligibly. Finally, SPRBFAO's load balance is quite stable in all domains, especially when all threads are invoked and perform search after a while. For example, its load balance ranges between 1.0051-1.064, 1.013-1.049, and 1.004-1.117 for grid ($i = 6$), pedigree ($i = 6$), and protein ($i = 2$), especially on those instances where SPRBFAO expands at least 1 mil-

lion nodes with 12 threads. Impact of parameter γ In Figure 3 we analyze the performance of SPRBFAO with 12 threads as a function of the parameter γ which controls the way different threads are encouraged or discouraged to start exploring a specific subproblem (see also Section 3). For this purpose and to better understand SPRBFAO’s scaling behavior, we ignore the heuristic compilation time. Therefore, we show the total search time (in seconds) over the instances that all parallel versions solve, and the search-time-based average speed-ups based on the instances where RBFAO needs at least 1 second to solve. We obtained these numbers for $\gamma \in \{0.001, 0.01, 0.1\}$. We see that all γ values lead to improved speed-ups. This is important because, unlike the approach of [8] which involves a sophisticated scheme, it is considerably simpler yet extremely efficient and only requires tuning a single parameter (γ). Of the three γ values, while SPRBFAO with $\gamma = 0.1$ spends the largest total search time, it yields the best speed-up. This indicates a trade-off about selecting γ . Since the instances used to calculate speed-up values are solved by RBFAO, they contain relatively easy instances. 7

Table 4: Total CPU time (sec) and node expansions for hard pedigree instances. SPRBFAO ran with 12 threads, $i = 20$ (type4b) and $i = 16$ (largeFam). Time limit 100 hours. instance

(n, k, w γ , h)					
type4b-100-19	type4b-120-17	type4b-130-21	type4b-140-19	largeFam3-10-52	
(7308,5,29,354)	(7766,5,24,319)	(8883,5,29,416)	(9274,5,30,366)	(1905,3,36,80)	
(mbe) time	400	191	281	488	13
RBFAO time nodes	132711	22243047591	210	4297063	290760
	51481315386				
248376	39920187143	154994	19363865449		
SPRBFAO time nodes	42846	50509174040	195	6046663	149321
	177393525747				
74643	85152364623	50700	44073583335		

On the other hand, several difficult instances solved by SPRBFAO with 12 threads are included in calculating the total search time. In case of $\gamma = 0.1$, because of increased search overhead, SPRBFAO needs more search time to solve these difficult instances. There is also one protein instance unsolved with $\gamma = 0.1$ but solved with $\gamma = 0.01$ and 0.001. This phenomenon can be explained as follows. With large γ , SPRBFAO searches in more diversified directions which could reduce lock contentions, resulting in improved speed-up values. However, due to larger diversification, when SPRBFAO with $\gamma = 0.1$ solves difficult instances, it might focus on less promising portions of the search space, resulting in increased total search time. Summary of the experiments In terms of search-time-based speed-ups, our parallel sharedmemory method SPRBFAO improved considerably over its sequential counterpart RBFAO, by up to 7 times using 12 threads. At relatively larger i -bounds, their corresponding computational overhead typically outweighed the gains obtained by parallel search. Still, parallel search had an advantage of solving additional instances unsolved by serial search. Finally, in Table 4 we report the results obtained on 5 very hard pedigree instances from [2] (mbe records the heuristic compilation time). We see again that SPRBFAO improved over RBFAO on all instances, while achieving a total-time-based speed-up of 3 on two of them

(i.e., type4b-100-19 and largeFam3-10-52).

5

Related Work

The distributed AOBB algorithm daoopt [8] which builds on the notion of parallel tree search [16], explores centrally the search tree up to a certain depth and solves the remaining conditioned sub-problems in parallel using a large grid of distributed processing units without a shared cache. In parallel evidence propagation, the notion of pointer jumping has been used for exact probabilistic inference. For example, Pennock [17] performs a theoretical analysis. Xia and Prasanna [18] split a junction tree into chains where evidence propagation is performed in parallel using a distributedmemory environment, and the results are merged later on. Proof-number search (PNS) in AND/OR spaces [19] and its parallel variants [20] have been shown to be effective in two-player games. As PNS is suboptimal, it cannot be applied as is to exact MAP inference. Kaneko [21] presents shared-memory parallel depth-first proof-number search with virtual proof and disproof numbers (vpdn). These combine proof and disproof numbers [19] and the number of threads examining a node. Thus, our $vq(n)$ is closely related to vpdn. However, vpdn has an over-counting problem, which we avoid due to the way we dynamically update $vq(n)$. Saito et al. [22] uses threads that probabilistically avoid the best-first strategy. Hoki et al. [23] adds small random values the proof and disproof numbers of each thread without sharing any cache table.

6

Conclusion

We presented SPRBFAOO, a new shared-memory parallel recursive best-first AND/OR search scheme in graphical models. Using the virtual q-values shared in a single cache table, SPRBFAOO enables threads to work on promising regions of the search space with effective reuse of the search effort performed by others. A homogeneous search mechanism across the threads achieves an effective load balancing without resorting to sophisticated schemes used in related work [8]. We prove the correctness of the algorithm. In experiments, SPRBFAOO improves considerably over current state-of-the-art sequential AND/OR search approaches, in many cases leading to considerable speed-ups (up to 7-fold using 12 threads) especially on hard problem instances. Ongoing and future research directions include proving the completeness conjecture, extending SPRBFAOO to distributed memory environments, and parallelizing the mini-bucket heuristic for shared and distributed memory. 8

2 References

- [1] R. Marinescu and R. Dechter. AND/OR branch-and-bound search for combinatorial optimization in graphical models. *Artificial Intelligence*, 173(16-17):1457-1491, 2009.
- [2] A. Kishimoto and R. Marinescu. Recursive best-first AND/OR search for optimization in graphical models. In *International Conference on Uncertainty in Artificial Intelligence (UAI)*, pages 400-409, 2014.
- [3] R.

Korf. Linear-space best-first search. *Artificial Intelligence*, 62(1):41?78, 1993.

[4] A. Kishimoto, A. Fukunaga, and A. Botea. Evaluation of a simple, scalable, parallel best-first search strategy. *Artificial Intelligence*, 195:222?248, 2013.

[5] Wahid Chrabakh and Rich Wolski. Gradsat: A parallel SAT solver for the Grid. Technical report, University of California at Santa Barbara, 2003.

[6] M. Campbell, A. Joseph Hoane Jr., and F.-h. Hsu. Deep Blue. *Artificial Intelligence*, 134(1? 2):57?83, 2002.

[7] M. Enzenberger, M. M?uller, B. Arneson, and R. Segal. FUEGO - an open-source framework for board games and Go engine based on Monte-Carlo tree search. *IEEE Transactions on Computational Intelligence and AI in Games*, 2(4):259?270, 2010.

[8] L. Otten and R. Dechter. A case study in complexity estimation: Towards parallel branch-and-bound over graphical models. In *Uncertainty in Artificial Intelligence (UAI)*, pages 665?674, 2012.

[9] J. Pearl. *Probabilistic Reasoning in Intelligent Systems*. Morgan Kaufmann, 1988.

[10] S. L. Lauritzen. *Graphical Models*. Clarendon Press, 1996.

[11] R. Dechter and R. Mateescu. AND/OR search spaces for graphical models. *Artificial Intelligence*, 171(2-3):73?106, 2007.

[12] R. Marinescu and R. Dechter. Memory intensive AND/OR search for combinatorial optimization in graphical models. *Artificial Intelligence*, 173(16-17):1492?1524, 2009.

[13] A. Nagai. *Dfn Algorithm for Searching AND/OR Trees and Its Applications*. PhD thesis, The University of Tokyo, 2002.

[14] M. Fishelson and D. Geiger. Exact genetic linkage computations for general pedigrees. *Bioinformatics*, 18(1):189?198, 2002.

[15] C. Yanover, O. Schueler-Furman, and Y. Weiss. Minimizing and learning energy functions for side-chain prediction. *Journal of Computational Biology*, 15(7):899?911, 2008.

[16] A. Grama and V. Kumar. State of the art in parallel search techniques for discrete optimization problems. *IEEE Transactions on Knowledge and Data Engineering*, 11(1):28?35, 1999.

[17] D. Pennock. Logarithmic time parallel Bayesian inference. In *Uncertainty in Artificial Intelligence (UAI)*, pages 431?438, 1998.

[18] Y. Xia and V. K. Prasanna. Junction tree decomposition for parallel exact inference. In *IEEE International Symposium on Parallel and Distributed Processing (IPDPS)*, 2008.

[19] L. V. Allis, M. van der Meulen, and H. J. van den Herik. Proof-number search. *Artificial Intelligence*, 66(1):91?124, 1994.

[20] A. Kishimoto, M. Winands, M. M?uller, and J.-T. Saito. Game-tree search using proof numbers: The first twenty years. *ICGA Journal*, Vol. 35, No. 3, 35(3):131?156, 2012.

[21] T. Kaneko. Parallel depth first proof number search. In *AAAI Conference on Artificial Intelligence*, pages 95?100, 2010.

[22] J.-T. Saito, M. H. M. Winands, and H. J. van den Herik. Randomized parallel proof-number search. In *Advances in Computers Games Conference (ACG?09)*, volume 6048 of *Lecture Notes in Computer Science*, pages 75?87. Springer, 2010.

[23] K. Hoki, T. Kaneko, A. Kishimoto, and T. Ito. Parallel dovetailing and its application to depthfirst proof-number search. *ICGA Journal*, 36(1):22?36, 2013.