Exact Solutions to NP-Complete Problems

Ref: - "Computer Algorithms", Horowitz, Sahni, Rajasekaran (Chapters 7, 8)
- Various texts on Combinatorial Algorithms or on Integer Linear Programming

Backtracking

• An organized exhaustive search which often avoids searching many possibilities

• The desired solution is often expressed as *n*-tuple, where the x_i's are chosen from some finite set S_i with $m_i = |S_i|$.

• The problem often requires finding one vector which maximizes, minimizes or satisfies a *criterion function* $P(x_1, x_2, ..., x_n)$.

• The *brute force* approach is to evaluate each of $m = m_1 m_2 ... m_n$ *n*-tuples from $S_1 \times S_2 \times ... \times S_n$ and identify the *n*-tuple yielding the optimal value.

• The basis idea of backtracking is to build the solution vector using *modified criterion function* $P_i(x_1, x_2, ..., x_i)$ to test whether the vector being formed have any chance of success.

• If a partial vector $(a_1, a_2, ..., a_i)$ has no chance of success, we avoid considering all of the $m_{i+1} m_{i+2} ... m_n$ possible test vectors $(a_1, a_2, ..., a_i, x_{i+1}, ..., x_n)$

• Many problems solved by backtracking satisfy a set of *constraints* which may divided into two categories: *explicit* and *implicit.*

• ***Explicit constraints*** are rules that restrict each x_i to take on values only from a given set

- examples: $x_i \geq 0$, $x_i = 0$ *or* 1, $l_i \leq x_i \leq u_i$
- depend on the particular instance *I* of the problem being solved
- the *n*-tuples that satisfy these conditions define a possible *solution space* for *I.*

• ***Implicit constraints*** are rules which the tuples in the solution space for I must satisfy in order to satisfy the criterion function.

• ***Example*** (8 Queens Problem)

- A classic problem in combinatorics is to place 8 queens on an 8 by 8 chessboard so that no two can "attack" each other (along a row, column, or diagonal).
- Since each queen (1-8) must be on a different row, we can assume queen *i* is on row *i.*
- All solutions to the 8-queens problem can be represented as an 8-tuple $(x_1, x_2, ..., x_8)$ where queen *i* is on column x_i.
- The explicit constraints are $S_i = \{1,2,...,8\}$, $1 \leq i \leq 8$. The solution space consists of 8^8 8-tuples.
- The implicit constraints are that no two x_i's can be the same (as queens must be on different columns) and no two queens can be on the same diagonal.
  - this implies that all solutions are permutations of the 8-tuple (1,2,…,8), and reduces the solution space from 8^8 tuples to 8! tuples.

• Backtracking algorithms determine problem solutions by systematically searching the solution space.

• Search is facilitated using a *tree organization* for the solution space.

• Many tree organizations may be possible for the same solution space.

• ***Example (n-Queens):*** *n* queens are placed on *n* by *n* chessboard so that no two attack (no two queens are on the same row, column, or diagonal).

• Generalizing earlier discussion, solution space contains all *n!* permutations of (1,2,…,n).

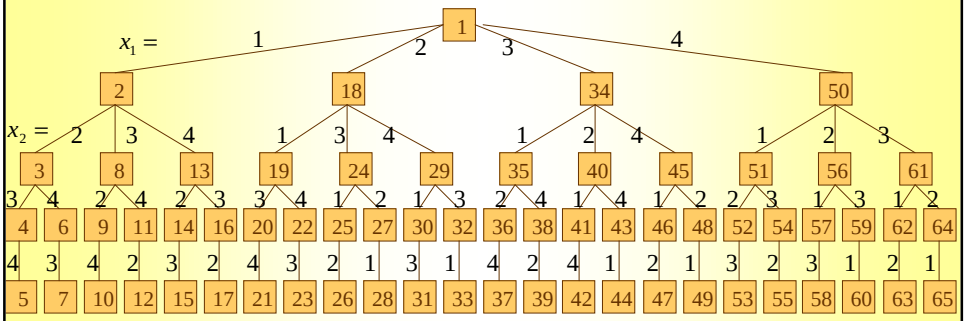
• The tree below shows possible organization for *n=4*.

• Tree is called a *permutation tree* (nodes are numbered as in *depth first search*).

• Edges labeled by possible values of x_i

• The *solution space* is all paths from the root node to a leaf node

• There are 4!=24 leaf nodes in tree



• ***Example (Sum of Subsets):*** Given positive numbers $w_i, 1 \le i \le n,$ and *m*, find all subsets of $\{w_1, w_2, ..., w_n\}$, whose sum is *m*.

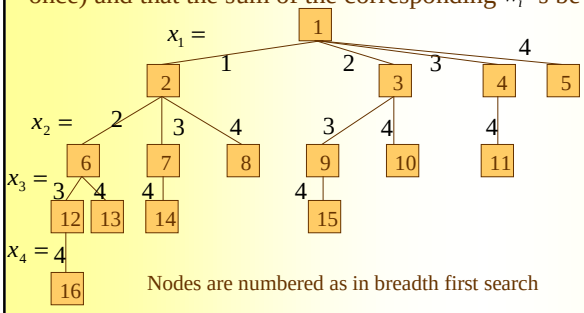
• If *n=4*, $\{w_1, w_2, w_3, w_4\}$ ={11,13,24,7} and *m*=31, the desired solution sets are (11,13,7) and (24,7).

• If the solution vectors are given using the indices of the w_i values used, then the solution vectors are (1,2,4) and (3,4).

• In general, all solutions are *k*-tuples $(x_1, x_2, ..., x_k)$ with $1 \le k \le n$ and different solutions may have different values of *k*.

• The *explicit constraints* on the solution space are that each $x_i \in \{1,2,...,n\}$.

• The *implicit constraints* are that $x_i < x_{i+1}, 1 \le i < n$, (so each item will occur only once) and that the sum of the corresponding w_i 's be *m*.



Nodes are numbered as in breadth first search

• The next figure gives the tree that corresponds to this variable tuple formation.

• An edge from a level *i* node to a level *i+1* node represents a value for x_i.

• The solution space is all paths from the root node to any node in the tree.

• Possible paths include *empty path*, (1), (1,2), (1,2,3), (1,2,3,4), (1,2,4), (1,3,4), …

• The leftmost subtree gives all subsets containing w_1, the next subtree gives all subsets containing w_2 but not w_1, etc

• ***Example (Sum of Subsets) again:*** Another formulation of this problem represents each solution by an *n*-tuple $(x_1, x_2, ..., x_n)$ with $x_i \in \{0,1\}, 1 \le i \le n$.

• Here $x_i = 0$ if w_i is not chosen and $x_i = 1$ if w_i is chosen.

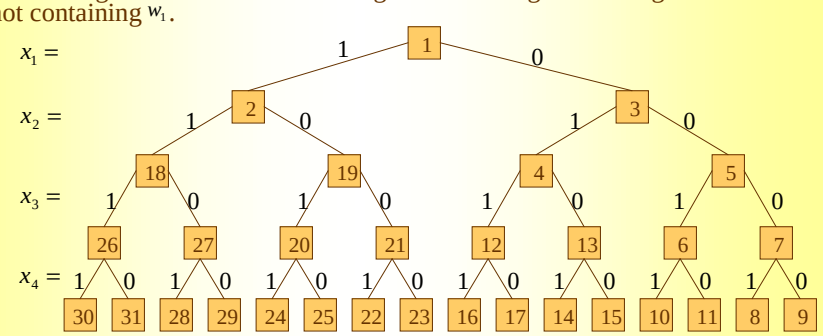
• Given the earlier instance of (11,13,24,7) and *m*=31, the solutions (11,13,7) and (24,7) are represented by (1,1,0,1) and (0,0,1,1).

• Here, all solutions have a fixed tuple size. The tree below corresponds to this formulation (nodes are numbered as in *D-search*).

• Edge from a level *i* node to a level *i+1* node is labeled with the value of x_i $(0 \text{ or } 1)$

• All paths from the root to a leaf give solution space.

• The left subtree gives all subsets containing w_1 and the right subtree gives all subsets not containing w_1.



Generating Problem States

• The two tree organizations for the sum of subsets problem are *static trees* (tree organization is independent of the problem instance being solved).

• Tree organizations that are problem instance dependent are called *dynamic trees* and are also used for some problems.

• Once a state space tree organization has been selected for a problem, the problem can be solved by
  - systematically generating the problem states,
  - finding which of these are solution states
  - finding which solution state are answer states

• A *live node* is a node which has been generated but whose children have not all been generated.

• An *E-node* (i.e., *expanding node*) is a live node whose children are currently being generated.

• A *dead node* is a generated node which is not to be expanded further or all of whose children have been generated.

• Two ways to generate problem states:
  - *Breadth First* Generation (queue of live nodes)
  - *Depth First* Generation (stack of live nodes)

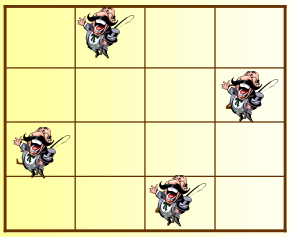
- *Depth First* Generation (stack of live nodes)
  - When a new child C of the current E-node R is generated, this child becomes the new E-node.
  - Then R will become the new E-node again when the subtree C has been fully explored.
  - Corresponds to a depth first search of the problem states.
- *Breadth First* Generation (queue of live nodes)
  - The E-node remains the E-node until it is dead.
- *Bounding functions* are used in both to kill live nodes without generating all of their children.
- At the end of the process, an answer node (or all answer nodes) are generated.
- The depth search generation method with bounding function is called *backtracking*.
- The breadth first generation method is used in the *branch-and-bound method*.

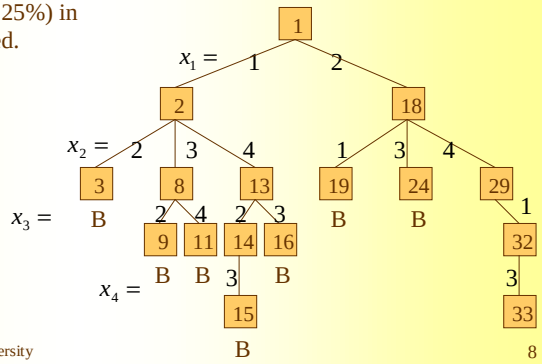
Example (backtracking on 4-queens problem)

- As a bounding function, use criterion that if $(x_1, x_2, ..., x_i)$ is the path to the current E-node, then some continuation $(x_1, x_2, ..., x_i, x_{i+1}, ..., x_n)$ exists that represents a chessboard without 2 queens attacking.
- Start with the root as the E-node. Then the path is ().
- The children of the E-nodes are generated in a left to right order.
- Node 2 is generated first and the path becomes (1). This corresponds to placing queen 1 on column 1.

Example (backtracking on 4-queens problem)

- Node 2 becomes the E-node, as no two queens are attacking.
- Node 3 is generated and is immediately killed, as queens 1 and 2 would be on a diagonal.
- Node 8 is generated and the path (1,3) is ok, so node 8 becomes the next E-node.
- Node 8 gets killed since none of its children can lead to a feasible chessboard.
- Backtrack to node 2 and generate another child, node 13, giving path (1,4) which is ok.
- The first child of node 13 is node 14, which gives path (1,4,2) and the feasible chessboard.
- This process continues, as indicated in the figure. The figure shows the portion of the state space tree we had on slide #3.
- Note that only 16 out of 65 nodes (or 25%) in the solution space are actually generated.





General Backtracking Algorithm

• This algorithm will find all answer nodes.

• If only the first solution is desired, a "flag" parameter can be added to indicate first success.

• Let $(x_1, x_2, ..., x_i)$ be a path from the root to a node in the state space tree.

• Let $T(x_1, x_2, ..., x_i)$ be the set of all possible values for x_{i+1} such that $(x_1, x_2, ..., x_i, x_{i+1})$ is also a path to a problem state (i.e., node).

• Let B_i be a boundary (Boolean) function such that if $B_i(x_1, x_2, ..., x_i)$ is false, then the path $(x_1, x_2, ..., x_i)$ cannot be extended to reach an answer node.

• Note that if $B_i(x_1, x_2, ..., x_i) = 1$, this does not guarantee that the path $(x_1, x_2, ..., x_i)$ can be extended to reach an answer node.

• Here is the recursive backtracking algorithm

```
Algorithm Backtrack(k)
for (each x[k] from T(x[1],x[2],…,x[k-1]) do
{ if (Bk (x[1],x[2],…,x[k])!= 0) then
    {if (x[1],x[2],…,x[k]) is a path to an answer node)
     then write (x[1..k]);
     if (k<n) then Backtrack(k+1);
    }
}
```

Comments

• the candidates for x[i+1] are values generated by T(x[1],x[2],…,x[i]) that satisfy B_{i+1}

• T( ) gives all candidates for x[1].

• elements are generated in a depth first manner, creating a preorder traversal (except for eliminated branches) of the state space tree.

• for many problems, the size of the state space tree is too large to permit generation of all nodes.

Efficiency of Backtracking

• The efficiency of a backtracking algorithm depends upon 4 factors
  • the time to generate the next x[k]
  • the number of x[k] choices that satisfy the explicit constraints
  • the time required to evaluate the bounding function B_i
  • the number of x[k] satisfying the B_i

• A good boundary function will drastically reduce the number of candidates that have to be considered.

• Often a tradeoff between bounding functions, as one that is good may take more time to evaluate.

• For many problems such as *n*-queens, no good bounding function are known.

• Rearrangement:
  • the principle of selecting the set S_i with fewest elements each time
  • since these sets can be taken in any order, smaller branching at the higher levels create larger subtrees
  • removal of early nodes cut off larger subtrees (see Fig. 7.7 in HSR)

• The first three factors that effect the time required for backtracking depend primarily on the state space tree organization selected

• Only the fourth factor may vary widely, depending on the problem instances.

- Worst case predictions for backtracking algorithms:
  - If the number of points in the solution space is 2^n or *n!* the worst case timing is usually either $O(p(n)2^n)$ or $O(p(n)\ n!)$, where $p(n)$ is a polynomial.
  - Backtracking can often solve some problem instances with large *n* in very small amounts of time. However, may be difficult to predict behavior of algorithm for particular problem instances.
- Estimating Nr. of nodes generated:
  - The number of nodes generated in a particular instance can be estimated using Monte Carlo methods
  - Starting at the top level, a random path is generated, as follows:
  - set *x* be a node on this path at level *i* of the state space tree; the boundary function B_i is used to determine the number m_i of its children which will be generated; one child is randomly selected, and the process continue until the path ends.
  - Then $m = m_1 + m_1m_2 + m_1m_2m_3 + \ldots$ is an estimate of the nodes that will be generated.
- Above estimate for *m* assumes the bounding functions are static and do not improve with time; It also assumes that the same boundary function is used for all nodes at the same level.
- The above two assumptions are not true for most backtracking algorithms; e.g., the boundary functions usually get stronger as information is gathered about the search.
- Consequently, the above value of *m* is likely to be high when these two assumptions are false.
- A better estimate would also result if the value *m* is the average returned for several (about 20) random paths.

Backtracking Algorithm for n-Queens problem

- Let $(x_1, x_2, \ldots, x_n)$ represent where the *i*th queen is placed (in row *i* and column x_i) on an *n* by *n* chessboard.
- Observe that two queens on the same diagonal that runs from "upper left" to "lower right" have the same "row-column" value.
- Also two queens on the same diagonal from "upper-right" to "lower left" have the same "row+column" value
- Then two queens at *(i,j)* and *(k,l)* are on the same diagonal if and only if

$$i-j=k-l \text{ or } i+j=k+l$$

iff

$$i-k=j-l \text{ or } j-l = k-i$$

iff

$$|j-l|=|i-k| .$$

- Algorithm PLACE(k,i) returns *true* if the *k*th queen can be placed in column *i* and runs in *O(k)* time (see next slide)
- Using PLACE, the recursive version of the general backtracking method can be used to give a precise solution to the n-queens problem
- Array *x[ ]* is global. Algorithm invoked by NQUEENS(1,n).

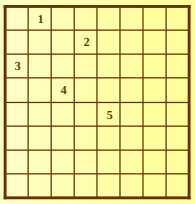
```
bool Place(int k, int i)
// Returns true if a queen can be placed in kth row and ith column. Otherwise it returns false.
// x[] is a global array whose first (k-1) values have been set.
// abs(r) returns the absolute value of r.
{
 for (int j=1; j < k; j++)
    if ((x[j] == i)            // Two in the same column
                  || (abs(x[j]-i) == abs(j-k)))    // or in the same diagonal
        return(false);
 return(true);
}

void NQueens(int k, int n)
// Using backtracking, this procedure prints all possible placements of n queens on an n x n
// chessboard so that they are nonattacking.
{
 for (int i=1; i<=n; i++) {
    if (Place(k, i)) {
       x[k] = i;
       if (k==n) { for (int j=1;j<=n;j++)
                        cout << x[j] << ' '; cout << endl;}
       else NQueens(k+1, n);
                  }
                        }
}
```


Efficiency of n-Queens over Brute Force

- For an 8x8 chessboard, there are $\binom{64}{8}$ ways to place 8 queens on the chessboard (billions of 8-tuples to examine)
- Requiring placement of queens on distinct rows and columns reduces the number of 8-tuples that must be examined to 8!= 40,320 8-tuples
- Next we estimate the number of nodes that will be generated by NQUEENS. The assumptions needed for this estimate hold for NQUEENS.
  - Boundary function is static
  - boundary functions does not change as search progress
  - additionally, nodes on the same level of the tree have the same degree
- Five trials using the ESTIMATE function described earlier are given on p.355 of HSR
  - each produces a random path and estimates the total number of nodes generated, based on this path
  - the average of these 5 estimates is 1625
  - the total number of nodes in the 8-queens state space tree is

$$1+\sum_{j=0}^{7}[\Pi_{i=0}^{j}(8-i)]=69,281$$

  - the estimated number of unbound nodes is only 2.34 % of the total number of nodes in the 8-queens state space tree.



(8,5,4,3,2)=1649

Sum of Subsets Algorithm Overview

• ***Problem Restated***: Given *n* distinct positive integers (called weights), find all combinations of these numbers whose sum is *m*.

• We use the state space tree based on the fixed tuple length $(w_1, w_2, ..., w_n)$ where $x_i = 0$ if w_i is not included and $x_i = 1$ if w_i is included (see Fig. on slide #5).

• The weights $(w_1, w_2, ..., w_n)$ are assumed to initially be sorted into increasing order.

• Note that the tree node corresponding to $(x_1, x_2, ..., x_k)$ cannot lead to an answer node unless

(1) $$\sum_{i=1}^{k} w_i x_i + \sum_{i=k+1}^{n} w_i \geq m$$

• Also, note that $(x_1, x_2, ..., x_k)$ cannot lead to an answer node unless

(2) $$\sum_{i=1}^{k} w_i x_i + w_{k+1} \leq m$$

• The boundary function used uses both of the preceding conditions:

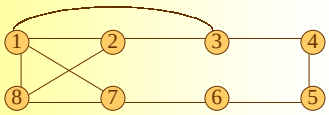
$B_k(x_1, x_2, ..., x_k) = true$ iff (1) and (2) hold

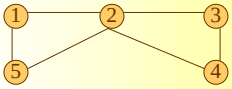
• The algorithm for the sum of subsets problem given in HSR is obtained by using this boundary function in the general recursive backtracking algorithm.

  • A couple of implementation simplifications used are explained in HSR (see pp. 358-9).

Hamiltonian Cycles Algorithm

• Example: Graph *G1* contains a Hamiltonian cycle 1,2,8,7,6,5,4,3,1 while graph *G2* contains no Hamiltonian cycle.

G1 = 

G2 = 

• The algorithm given works on both directed and undirected graphs

• All distinct cycles will be found.

• Each x_i in the backtracking solution vector $(x_1, x_2, ..., x_n)$ represents the *i*th vertex visited in the proposed cycle

• The vertices of the graph are assumed to be named using the first *n* positive integers.

• To avoid printing the same cycle *n* times, we require $x_1 = 1$

• The algorithm *NextValue* determines a possible next vertex for the proposed cycle

  • if $1<k<n$, then x_k can be any vertex *v* that is distinct from $x_1, x_2, ..., x_{k-1}$ and is connected by an edge to x_{k-1}

  • the vertex x_n must be one remaining vertex and must be connected by an edge to both x_1 and x_{n-1}

• The backtracking algorithm *Hamiltonian(k)* is obtained by using *NextValue* to select a legal vertex to add. No boundary function is used.

- The main algorithm starts by
  - initializing the adjacency matrix *G[1:n,1:n]*
  - setting *x[2:n]=0*
  - setting *x[1]=1*
  - executing *Hamiltonian(2)*

Recursive algorithm that finds all Hamiltonian cycles →

```
void Hamiltonian(int k)
  // This program uses the recursive formulation of
  // backtracking to find all the Hamiltonian cycles
  // of a graph. The graph is stored as an adjacency
  // matrix G[1:n][1:n]. All cycles begin at node 1.
  {
     do { // Generate values for x[k].
        NextValue(k);  // Assign a legal next value to x[k].
        if (!x[k]) return;
        if (k == n) {
           for (int i=1; i<=n; i++) cout << x[i] << ' ';
           cout << "1\n";
                    }
        else Hamiltonian(k+1);
          } while (1);
   }
```



```
void NextValue(int k)
  // x[1],...,x[k-1] is a path of k-1 distinct vertices.
  // If x[k]==0, then no vertex has as yet
  // been assigned to x[k]. After execution x[k] is assigned
  // to the lowest numbered vertex which
  // i) does not already appear in x[1],x[2],...,x[k-1]; and
  // ii) is connected by an edge to x[k-1].
  // Otherwise x[k]==0.
  // If k==n, then in addition x[k] is connected to x[1].
  {do {
        x[k] = (x[k]+1) % (n+1); // Next vertex
        if (!x[k]) return;
        if (G[x[k-1]][x[k]]) { // Is there an edge?
          for (int j=1; j<=k-1; j++) if (x[j]==x[k]) break;
                          // Check for distinctness.
          if (j==k) // If true, then the vertex is distinct.
            if ((k<n) || ((k==n) && G[x[n]][x[1]]))
              return;
                                  }
       } while(1);
  }
```

Returning at this line causes *Hamiltonian(k)* to backtrack

Assigns *x[k]* the values 1,2,…,n successively, following failure at

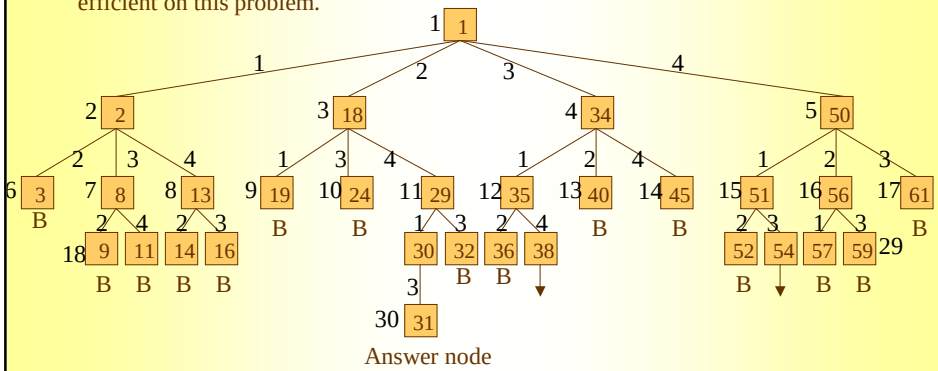
Homework problem:

Generalize *Hamiltonian* so that it processes a graph whose edges have cost associated with them and finds a Hamiltonian cycle with minimum cost. You can assume that all edge costs are positive (Ex. 3, p. 368 of HSR)

Branch and Bound Algorithms

- Refers to all state space search methods in which all children of the E-nodes are generated before any other live nodes become E-nodes.
- ***Breadth Fist Search*** (BFS) will be called FIFO (fist in, first out)
  - each new node is placed in a queue
  - after all children of current E-node are generated, the node at front of queue become the E-node.
- ***D-search*** will be called a LIFO (last in, first out)
  - new nodes are placed in stack
- As with backtracking, bounding functions will be used to avoid generating trees with no answer node.
- ***Example:*** 4 Queen FIFO Branch & Bound Algorithm.
  - The state space tree in Fig. on slide #3 is used, so node numbers do not indicate order of generation.
  - Initially, only the root node is alive (no queens placed)
  - Expanding the root E-node generates its children nodes in the order 2,18,34, and 50. These nodes represent a 4x4 chessboard with queen 1 in row 1 and columns 1,2,3, and 4 respectively.
  - The only live nodes are now 1,18,34,50, and the next E-node is 2. It is expanded, generating nodes 3,8,13.

- Node 3 is killed immediately by the bounding function used in backtracking algorithm and nodes 8,13 are added to queue of live nodes.
- This process is continued, generating below figure.
- Comparing the two trees of generated nodes, it is clear that backtracking is more efficient on this problem.



Least Cost (LC) search

- Both FIFO and LIFO are rigid and blind.
- The search for an answer node can often be speeded up using an "intelligent" ranking function *C( )* for the live nodes.

Least Cost (LC) search

• In 4-Queens example, if *C( )* had assigned node 30 a better rank than other live nodes, it would have become the E-node following node 29.

• An ideal way to assign rank to each live node *x* is the number of levels the nearest answer node (in the subtree with root *x*) is from *x*.

• Using this ranking function on the previous 4-queens example would have assigned rank 1 to both answer nodes 30 and 38.

• Let *g(x)* be an estimate of the additional effort needed to reach an answer node from *x*.

• Node *x* is assigned a rank using a function *C( )* defined by $C(x)=f(h(x))+g(x)$, where *h(x)* is the cost of reaching *x* from the root.
f is a non-decreasing weight function.

• The use of nonzero *f* helps prevent the search algorithm from making unnecessarily deep probes into the search tree.

• A nonzero *f* is needed, as otherwise a child *y* of the current E-node *x* will become the next E-node since $g(y) \leq g(x)$ and *x* had the previous lowest rank.

• Use of non-zero *f* forces the search algorithm to favor nodes closer to the root, reducing the probability of a deep and fruitless search into the tree.

• A search that uses a cost function *C( )* to choose the next E-node to be a live node with minimum *C( )* value is called a ***LC-search***.

• If $g=0$, $f=1$, and *h(x)* is the level of node *x*, this LC-search is a BFS algorithms which generates nodes by levels.

• If $f=0$ and $g(y)<g(x)$ when *y* is a child of *x*, this LC-search is a D-search.

• The *cost function c( )* is defined as follows

  • if *x* is an answer node, then *c(x)* is the cost of reaching *x* from the root of the state space tree.

  • if *x* is not an answer node, but the subtree of *x* contains an answer node, then c*(x)* is the minimal cost of an answer node in subtree *x*.

  • otherwise, $c(x)=\infty$

• Then, *C( )* with $f=1$, that is, $C(x)=h(x)+g(x)$, is an estimate of *c( )*.

• *C( )* should be chosen so that it is easy to compute. It will normally have the additional property that if *x* is an answer node or leaf node, then $c(x)=C(x)$.

Least Cost Search Algorithm

• This algorithm assumes two additional algorithms, *Least(x)* and *Add(x)* to manage the list of live nodes.

• *Least( )* finds a live node with least *C( )* value. This node is deleted from the list of live nodes and returned.

• *Add(x)* adds the new live node *x* to the list of live nodes.

• With each node *x* that becomes alive, we associate a field *parent* which stores the parent of *x*.

Least Cost Search Algorithm

• This allows LC-search to output a path from the answer node it finds to the root node.

• LC-search terminates only when either an answer node is found or the entire state space tree has been generated and searched.

• Note that termination is only guaranteed for finite space trees.

• It is advisable to restrict the search in LC-search to find answer nodes with costs not exceeding a given bound ***C***.

• Note: *Least* and *Add* can be defined to implement a stack or queue as well, so the algorithms for LC, FIFO, and LIFO search are essentially the same.

```
struct listnode {struct listnode *next, *parent; float cost;};
LCSearch(struct listnode *t)   // Search t for an answer node.
{   Struct listnode *x, *E, *Least( );
    if (*t is an answer node) output *t and return;
    E=t;  // E-node
    initialize the list of live nodes to be empty;
    do  { for (each child x of E)   {
                if (x is an answer node) output the path from x to t and return;
                Add(x);   // x is a new live node.
                x→parent = E; //  pointer for path to root
                                    }
          if there are no more live nodes) {count << "No answer node\n";  return; }
          E=Least( );
        }  while(1);
}
```


Dynamic Programming

• This is another technique for finding exact solutions to NP-Complete problems.

• Examples:

  • 0/1 Knapsack Problem (your old homework problem; $O(nW)$ time algorithm)

  • Traveling Salesman Problem (HSR p. 298)

READ (in HSR) Sections: 7.1-7.3, 7.5, and 8.1(8.1.1-8.1.3).

Homework 7:

• **Problems:**

  • no more problems at this moment