Backtracking

General method

- Useful technique for optimizing search under some constraints
- Express the desired solution as an $n$-tuple $(x_1, \ldots, x_n)$ where each $x_i \in S_i$, $S_i$ being a finite set
- The solution is based on finding one or more vectors that maximize, minimize, or satisfy a criterion function $P(x_1, \ldots, x_n)$
- Sorting an array $a[n]$
  - Find an $n$-tuple where the element $x_i$ is the index of $i$th smallest element in $a$
  - Criterion function is given by $a[x_i] \leq a[x_{i+1}]$ for $1 \leq i < n$
  - Set $S_i$ is a finite set of integers in the range $[1,n]$
- Brute force approach
  - Let the size of set $S_i$ be $m_i$
  - There are $m = m_1m_2 \cdots m_n$ $n$-tuples that satisfy the criterion function $P$
  - In brute force algorithm, you have to form all the $m$ $n$-tuples to determine the optimal solutions by evaluating against $P$
- Backtrack approach
  - Requires less than $m$ trials to determine the solution
  - Form a solution (partial vector) one component at a time, and check at every step if this has any chance of success
  - If the solution at any point seems not-promising, ignore it
  - If the partial vector $(x_1, x_2, \ldots, x_i)$ does not yield an optimal solution, ignore $m_{i+1} \cdots m_n$ possible test vectors even without looking at them
  - Effectively, find solutions to a problem that incrementally builds candidates to the solutions, and abandons each partial candidate that cannot possibly be completed to a valid solution
    * Only applicable to problems which admit the concept of partial candidate solution and a relatively quick test of whether the partial solution can grow into a complete solution
    * If a problem does not satisfy the above constraint, backtracking is not applicable
      - Backtracking is not very efficient to find a given value in an unordered list
- All the solutions require a set of constraints divided into two categories: explicit and implicit constraints

**Definition 1** Explicit constraints are rules that restrict each $x_i$ to take on values only from a given set.

- Explicit constraints depend on the particular instance $I$ of problem being solved
- All tuples that satisfy the explicit constraints define a possible solution space for $I$
- Examples of explicit constraints
  * $x_i \geq 0$, or all nonnegative real numbers
  * $x_i = \{0, 1\}$
  * $l_i \leq x_i \leq u_i$

**Definition 2** Implicit constraints are rules that determine which of the tuples in the solution space of $I$ satisfy the criterion function.

- Implicit constraints describe the way in which the $x_i$s must relate to each other.
Determine problem solution by systematically searching the solution space for the given problem instance
  – Use a tree organization for solution space

8-queens problem
  – Place eight queens on an 8 × 8 chessboard so that no queen attacks another queen
    * A queen attacks another queen if the two are in the same row, column, or diagonal

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  – Identify data structures to solve the problem
    * First pass: Define the chessboard to be an 8 × 8 array
    * Second pass: Since each queen is in a different row, define the chessboard solution to be an 8-tuple \((x_1, \ldots, x_8)\), where \(x_i\) is the column for \(i\)th queen

  – Identify explicit constraints
    * Explicit constraints using 8-tuple formulation are \(S_i = \{1, 2, 3, 4, 5, 6, 7, 8\}, 1 \leq i \leq 8\)
    * Solution space of \(8^8\) 8-tuples

  – Identify implicit constraints
    * No two \(x_i\) can be the same, or all the queens must be in different columns
      - All solutions are permutations of the 8-tuple \((1, 2, 3, 4, 5, 6, 7, 8)\)
      - Reduces the size of solution space from \(8^8\) to \(8!\) tuples
    * No two queens can be on the same diagonal
  – The solution above is expressed as an 8-tuple as \((4, 6, 8, 2, 7, 1, 3, 5)\)

Sum of subsets
  – Given \(n\) positive numbers \(w_i, 1 \leq i \leq n\), and \(m\), find all subsets of \(w_i\) whose sums are \(m\)
  – For example, \(n = 4, w = (11, 13, 24, 7)\), and \(m = 31\), the desired subsets are \((11, 13, 7)\) and \((24, 7)\)
  – The solution vectors can also be represented by the indices of the numbers as \((1, 2, 4)\) and \((3, 4)\)
    * All solutions are \(k\)-tuples, \(1 \leq k \leq n\)

  – Explicit constraints
    * \(x_i \in \{j \mid j \text{ is an integer and } 1 \leq j \leq n\}\)
  – Implicit constraints
    * No two \(x_i\) can be the same
    * \(\sum w_{x_i} = m\)
    * \(x_i < x_{i+1}, 1 \leq i < k\) (total order in indices)
      - Helps in avoiding the generation of multiple instances of same subset; \((1, 2, 4)\) and \((1, 4, 2)\) are the same subset
  – A better formulation of the problem is where the solution subset is represented by an \(n\)-tuple \((x_1, \ldots, x_n)\) such that \(x_i \in \{0, 1\}\)
    * The above solutions are then represented by \((1, 1, 0, 1)\) and \((0, 0, 1, 1)\)
Backtracking

– For both the above formulations, the solution space is $2^n$ distinct tuples

• $n$-queen problem
  – A generalization of the 8-queen problem
  – Place $n$ queens on an $n \times n$ chessboard so that no queen attacks another queen
  – Solution space consists of all $n!$ permutations of the $n$-tuple $(1, 2, \ldots, n)$
  – Permutation tree with 4-queen problem
    * Represents the entire solution space
    * $n!$ permutations for the $n$-tuple solution space
    * Edges are labeled by possible values of $x_i$
    * Solution space is defined by all paths from root to leaf nodes
    * For 4-queen problem, there are $4! = 24$ leaf nodes in permutation tree

• Sum of subsets problem
  – Possible tree organizations for the two different formulations of the problem
    – Variable tuple size formulation
      * Edges labeled such that an edge from a level $i$ node to a level $i + 1$ node represents a value for $x_i$
      * Each node partitions the solution space into subsolution spaces
      * Solution space is defined by the path from root node to any node in the tree
    – Fixed tuple size formulation
      * Edges labeled such that an edge from a level $i$ node to a level $i + 1$ node represents a value for $x_i$ which is either 0 or 1
      * Solution space is defined by all paths from root node to a leaf node
      * Left subtree defines all subsets containing $w_1$; right subtree defines all subsets not containing $w_1$
      * $2^n$ leaf nodes representing all possible tuples

• Terminology
  **Problem state** is each node in the depth-first search tree
  **State space** is the set of all paths from root node to other nodes
  **Solution states** are the problem states $s$ for which the path from the root node to $s$ defines a tuple in the solution space
    – In variable tuple size formulation tree, all nodes are solution states
    – In fixed tuple size formulation tree, only the leaf nodes are solution states
    – Partitioned into disjoint sub-solution spaces at each internal node
  **Answer states** are those solution states $s$ for which the path from root node to $s$ defines a tuple that is a member of the set of solutions
    – These states satisfy implicit constraints
  **State space tree** is the tree organization of the solution space
  **Static trees** are ones for which tree organizations are independent of the problem instance being solved
    – Fixed tuple size formulation
    – Tree organization is independent of the problem instance being solved
  **Dynamic trees** are ones for which organization is dependent on problem instance
    – After conceiving state space tree for any problem, the problem can be solved by systematically generating problem states, checking which of them are solution states, and checking which solution states are answer states
  **Live node** is a generated node for which all of the children have not been generated yet
**E-node** is a live node whose children are currently being generated or explored

**Dead node** is a generated node that is not to be expanded any further

- All the children of a dead node are already generated
- Live nodes are killed using a **bounding function** to make them dead nodes

- **Depth-first search**
  - As soon as a new child $C$ of the current $E$-node $P$ is generated, $C$ becomes the new $E$-node; $P$ becomes the $E$-node again when the subtree for $C$ is fully explored

- **Backtracking is depth-first node generation with bounding functions**

- **Backtracking on 4-queens problem**
  - Bounding function
    - If $(x_1, x_2, \ldots, x_i)$ is the path to the current $E$-node, then all children nodes with parent-child labelings $x_{i+1}$ are such that $(x_1, \ldots, x_{i+1})$ represents a chessboard configuration in which no two queens are attacking
    - Start with root node as the only live node, making it $E$-node and with path ()
    - Generate children in ascending order
    - If the new node does not evaluate properly with the bounding function, it is immediately killed

- **Backtracking process**
  - Assume that all answer nodes are to be found and not just one
  - Let $(x_1, x_2, \ldots, x_i)$ be the path from root to a node in the state space tree
  - Let $T(x_1, x_2, \ldots, x_i+1)$ be the set of all possible values for $x_{i+1}$ such that $(x_1, x_2, \ldots, x_{i+1})$ is also a path to a problem state
  - $T(x_1, x_2, \ldots, x_n) = \emptyset$
  - Assume a bounding function $B_{i+1}$ expressed as a predicate such that if $B_{i+1}(x_1, x_2, \ldots, x_{i+1})$ is false for a path $(x_1, x_2, \ldots, x_{i+1})$ from root to a problem state, then the path cannot be extended to reach an answer node

```
algorithm backtrack ( k )
// Describes a backtracking process using recursion
// Input: First k-1 values x[1], x[2], ..., x[k-1] of the solution vector
// x[1:n] have been assigned
// x and n are global
// Invoked by backtrack ( 1 );
{
  for each x[k] in T(x[1], ..., x[k-1])
  {
    if ( B_k(x[1], x[2], ..., x[k]) != 0 )
    {
      if ( x[1], x[2], ..., x[k] is a path to an answer node )
        write ( x[1:k] );
      if ( k < n )
        backtrack ( k + 1 );
    }
  }
}
```

- All possible elements for $k$th position of the tuple that satisfy $B_k$ are generated one by one and attached to the current vector $(x_1, \ldots, x_{k-1})$
- Each time $x_k$ is attached, we check whether a solution has been found
- When the for loop exits, no more values for $x_k$ exist and the current copy of backtrack ends
* The last unresolved call resumes; the one that continues to examine remaining elements assuming only \( k - 2 \) values have been set
* The algorithm can be modified to quit if just a single solution is found

- Iterative backtracking algorithm

```plaintext
algorithm ibacktrack ( n )
// Iterative backtracking process
// All solutions are generated in x[1:n] and printed as soon as they are found
{
    k = 1;
    while ( k != 0 )
    {
        if ( there remains an untried x[k] in T(x[1], x[2], ..., x[k-1])
            and B_k( x[1], ..., x[k] ) is true )
        {
            if ( x[1], ..., x[k] is a path to an answer node )
                write ( x[1:k] );
            k = k + 1;  // Consider the next set
        }
        else
        {
            k = k - 1;  // Backtrack to the previous set
        }
    }
}
```