Informed Search

Chapter 3.5 – 3.6, 4.1

Informed Search

• Informed searches use domain knowledge to guide selection of the best path to continue searching

• Heuristics are used, which are informed guesses

• Heuristic means "serving to aid discovery"

Informed Search

• Define a heuristic function, $h(n)$
  – uses domain-specific information in some way
  – is computable from the current state description
  – it estimates
    • the "goodness" of node $n$
    • how close node $n$ is to a goal
    • the cost of minimal cost path from node $n$ to a goal state

Informed Search

• $h(n) \geq 0$ for all nodes $n$

• $h(n)$ close to 0 means we think $n$ is close to a goal state

• $h(n)$ very big means we think $n$ is far from a goal state

• All domain knowledge used in the search is encoded in the heuristic function, $h$

• An example of a “weak method” for AI because of the limited way that domain-specific information is used to solve a problem
Best-First Search

- Sort nodes in the Frontier list by increasing values of an evaluation function, \( f(n) \), that incorporates domain-specific information.

- This is a generic way of referring to the class of informed search methods.

Greedy Best-First Search

- Use as an evaluation function, \( f(n) = h(n) \), sorting nodes in the Frontier list by increasing values of \( f \).

- Selects the node to expand that is believed to be closest (i.e., smallest \( f \) value) to a goal node.

Greedy Best-First Search

\[
 f(n) = h(n) \\
\text{# of nodes tested: 0, expanded: 0} \\
\begin{array}{|c|c|}
\hline
\text{expnd. node} & \text{Frontier list} \\
\hline
S & (S:B) \\
\hline
\end{array}
\]

Greedy Best-First Search

\[
 f(n) = h(n) \\
\text{# of nodes tested: 1, expanded: 1} \\
\begin{array}{|c|c|}
\hline
\text{expnd. node} & \text{Frontier list} \\
\hline
S & (S:B) \\
\hline
A & (S,B) \\
\hline
\end{array}
\]
Greedy Best-First Search

- Fast but not optimal

# of nodes tested: 3, expanded: 2

expnd. node | Frontier list
---|---
S | (C:3, B:4, A:8)
C | not goal (G:0, B:4, A:8)

\[ f(n) = h(n) \]

Greedy Best-First Search

Not complete
- Not optimal/admissible

Greedy search finds the left goal (solution cost of 7)
Optimal solution is the path to the right goal (solution cost of 5)
**Beam Search**
- Use an evaluation function $f(n) = h(n)$ as in greedy best-first search, and restrict the maximum size of the Frontier to a constant, $k$
- Only keep $k$ best nodes as candidates for expansion, and throw away the rest
- More space efficient than Greedy Search, but may throw away a node on a solution path
- Not complete
- Not optimal/admissible

**Algorithm A Search**
- Use as an evaluation function $f(n) = g(n) + h(n)$, where $g(n)$ is minimal cost path from start to current node $n$ (as defined in UCS)
- The $g$ term adds a “breadth-first component” to the evaluation function
- Nodes on the Frontier are ranked by the estimated cost of a solution, where $g(n)$ is the cost from the start node to node $n$, and $h(n)$ is the estimated cost from node $n$ to a goal

**Algorithm A* Search**
- Use the same evaluation function used by Algorithm A, except add the constraint that for all nodes $n$ in the search space, $h(n) \leq h^*(n)$, where $h^*(n)$ is the actual cost of the minimum-cost-path from $n$ to a goal
- The cost to the nearest goal is never over-estimated
- When $h(n) \leq h^*(n)$ holds true for all $n$, $h$ is called an admissible heuristic function
- An admissible heuristic guarantees that a node on the optimal path cannot look so bad so that it is never considered

**Is Algorithm A Optimal?**

- $h(A) = 6$, $g(S) = 1$, $g(G) = 0$, $h(S) = 7$, $h(G) = 0$
- $f(S) = g(S) + h(S) = 1 + 7 = 8$
- $f(A) = g(A) + h(A) = 1 + 6 = 7$
- $f(G) = g(G) + h(G) = 0 + 0 = 0$

Since $f(S) > f(A) > f(G)$, $S$ is not expanded, and the algorithm is not optimal.
Admissible Heuristics are Good for Playing *The Price is Right*

**Algorithm A* Search**

- Complete
- Optimal / Admissible

**Example**

<table>
<thead>
<tr>
<th>n</th>
<th>g(n)</th>
<th>h(n)</th>
<th>f(n)</th>
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<tbody>
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<td>S</td>
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</table>

\(g(n)\) = actual cost to get to node \(n\) from start

<table>
<thead>
<tr>
<th>n</th>
<th>g(n)</th>
<th>h(n)</th>
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$g(n) = \text{actual cost to get to node } n \text{ from start}$

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\[ g(n) = \text{actual cost to get to node } n \] from start

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</tbody>
</table>

\[ h(n) = \text{estimated cost to get to a goal} \] from node n

Example

<table>
<thead>
<tr>
<th>n</th>
<th>g(n)</th>
<th>h(n)</th>
<th>f(n)</th>
<th>h*(n)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S</td>
<td>0</td>
<td>8</td>
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<td>A</td>
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<td>B</td>
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<tr>
<td>C</td>
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<tr>
<td>G</td>
<td>10/9/13</td>
<td>0</td>
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</tr>
</tbody>
</table>

\[ f(n) = g(n) + h(n) \] actual cost to get from start to n plus estimated cost from n to goal

Example

<table>
<thead>
<tr>
<th>n</th>
<th>g(n)</th>
<th>h(n)</th>
<th>f(n)</th>
<th>h*(n)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S</td>
<td>0</td>
<td>8</td>
<td>8</td>
<td></td>
</tr>
<tr>
<td>A</td>
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</table>

\[ h(n) = \text{estimated cost to get to a goal} \] from node n
Example

\[
\begin{array}{|c|c|c|c|c|}
\hline
n & g(n) & h(n) & f(n) & h^*(n) \\
\hline
S & 0 & 8 & 8 \\
A & 1 & 8 & 9 \\
B & 5 & 4 & 9 \\
C & 8 & 3 & 11 \\
D & 4 & = & = \\
E & 8 & = & = \\
G & 10/9/13 & 0 & 10/9/13 \\
\hline
\end{array}
\]

\[h^*(n) = \text{true cost of minimal path from } n \text{ to a goal}\]

Example

\[
\begin{array}{|c|c|c|c|c|c|}
\hline
n & g(n) & h(n) & f(n) & h^*(n) \\
\hline
S & 0 & 8 & 8 & 9 \\
A & 1 & 8 & 9 & 9 \\
B & 5 & 4 & 9 & 4 \\
C & 8 & 3 & 11 & 4 \\
D & 4 & = & = & = \\
E & 8 & = & = & = \\
G & 10/9/13 & 0 & 10/9/13 & 0 \\
\hline
\end{array}
\]

\[h^*(n) = \text{true cost of minimal path from } n \text{ to a goal}\]
$h^*(n)$ = true cost of minimal path from $n$ to a goal

Since $h(n) \leq h^*(n)$ for all $n$, $h$ is admissible.
Admissible Heuristic Functions, $h$

- 8-Puzzle example

<table>
<thead>
<tr>
<th>Example State</th>
<th>Goal State</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 5 2</td>
<td>1 2 3</td>
</tr>
<tr>
<td>6 3 7</td>
<td>4 5 6</td>
</tr>
<tr>
<td>4 8 7</td>
<td>7 8</td>
</tr>
</tbody>
</table>

- Which of the following are admissible heuristics?

\[ h(n) = \text{number of tiles in wrong position} \]
\[ h(n) = 0 \]
\[ h(n) = 1 \]
\[ h(n) = \text{sum of “City-block distance” between each tile and its goal location} \]

Note: City-block distance = $L_1$ norm

Admissible Heuristic Functions, $h$

Which of the following are admissible heuristics?

\[ h(n) = h^*(n) \]
\[ h(n) = \max(2, h^*(n)) \]
\[ h(n) = \min(2, h^*(n)) \]
\[ h(n) = h^*(n) - 2 \]
\[ h(n) = \sqrt{h^*(n)} \]

A* Revisiting States

- One more complication: A* might visit an expanded state (on Frontier or Expanded), and discover a better path

<table>
<thead>
<tr>
<th>S</th>
<th>C</th>
<th>B</th>
<th>G</th>
</tr>
</thead>
<tbody>
<tr>
<td>h=2</td>
<td>h=2</td>
<td>h=1</td>
<td>h=0</td>
</tr>
</tbody>
</table>

When should A* Stop?

- A* should terminate only when a goal is removed from the priority queue

<table>
<thead>
<tr>
<th>S</th>
<th>B</th>
<th>C</th>
<th>G</th>
</tr>
</thead>
<tbody>
<tr>
<td>h=2</td>
<td>h=1</td>
<td>h=1</td>
<td>h=0</td>
</tr>
</tbody>
</table>

- Same rule as for uniform cost search
- A* with $h() = 0$ is uniform cost search

<table>
<thead>
<tr>
<th>S</th>
<th>D</th>
<th>C</th>
<th>G</th>
</tr>
</thead>
<tbody>
<tr>
<td>h=1</td>
<td>h=1</td>
<td>h=1</td>
<td>h=0</td>
</tr>
</tbody>
</table>

- Solution: Put D back into the priority queue, with the smaller $g$ value
A* Algorithm for General State-Space Graphs

Frontier = \{S\} where \(S\) is the start node
Explored = \{

Loop do
  if Frontier is empty then return failure
  pick node, \(n\), with min \(f\) value from Frontier
  if \(n\) is a goal node then return solution
  foreach each child, \(n'\), of \(n\) do
    if \(n'\) not in Explored or Frontier
      then add \(n'\) to Frontier
    else if \(g(n') \geq g(m)\) then throw \(n'\) away
      else add \(n'\) to Frontier and remove \(m\)
  Remove \(n\) from Frontier and add \(n\) to Explored

Note: \(m\) is the node in Frontier or Explored that is the same state as \(n'\)

Consistency

- A heuristic, \(h\), is called consistent or monotonic if, for every node \(n\) and every successor \(n'\) of \(n\), the estimated cost of reaching the goal from \(n\) is no greater than the step cost of getting to \(n'\) plus the estimated cost of reaching the goal from \(n'\):
  \[c(n, n') \geq h(n) - h(n')\]
  or, equivalently: \(h(n) \leq c(n, n') + h(n')\)
- Triangle inequality for heuristics
- Values of \(f(n)\) along any path are nondecreasing
- When a node is selected for expansion by A*, the optimal path to that node has been found

A* Search

\(f(n) = g(n) + h(n)\)
# of nodes tested: 0, expanded: 0

<table>
<thead>
<tr>
<th>expnd. node</th>
<th>Frontier list</th>
</tr>
</thead>
<tbody>
<tr>
<td>(S:0+8)</td>
<td></td>
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</tbody>
</table>

Note: \(h\) is admissible and consistent

A* Search

\(f(n) = g(n) + h(n)\)
# of nodes tested: 1, expanded: 1

<table>
<thead>
<tr>
<th>expnd. node</th>
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</tr>
</thead>
<tbody>
<tr>
<td>(S:8)</td>
<td>(S)</td>
</tr>
<tr>
<td>(A:5+B:8+C:3)</td>
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</tbody>
</table>

Note: \(h\) is admissible and consistent
A* Search

\[ f(n) = g(n) + h(n) \]

# of nodes tested: 4, expanded: 3

<table>
<thead>
<tr>
<th>expnd. node</th>
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<tbody>
<tr>
<td>S</td>
<td>(S: 8)</td>
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<tr>
<td>A</td>
<td>(A: 9, B: 9, C: 11)</td>
</tr>
<tr>
<td>B</td>
<td>(B: 9, G: 10, C: 11, D: (\infty), E: (\infty))</td>
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<tr>
<td>C</td>
<td>(C: 11, D: (\infty), E: (\infty))</td>
</tr>
</tbody>
</table>

Not expanded.

- Pretty fast and optimal
- Path: S, B, G
- Cost: 9
Proof of A* Optimality (by Contradiction)

• Let $G$ be the goal in the optimal solution
  $G2$ be a sub-optimal goal found using A* where $f(n) = g(n) + h(n)$, and $h(n)$ is admissible
  $f^*$ be the cost of the optimal path from Start to $G$
• Hence $g(G2) > f^*$
  That is, A* found a sub-optimal path (which it shouldn't)

Proof of A* Optimality (by Contradiction)

• Let $n$ be some node on the optimal path but not on the path to $G2$
  $f(n) \leq f^*$
  by admissibility, since $f(n)$ never overestimates the cost to the goal it must be ≤ the cost of the optimal path
• $f(G2) \leq f(n)$
  $G2$ was chosen over $n$ for the sub-optimal goal to be found
• $f(G2) \leq f^*$
  combining equations

Proof of A* Optimality (by Contradiction)

• $f(G2) \leq f^*$
• $g(G2) + h(G2) \leq f^*$
  substituting the definition of $f$
• $g(G2) \leq f^*$
  because $h(G2) = 0$ since $G2$ is a goal node
• This contradicts the assumption that $G2$ was sub-optimal, $g(G2) > f^*$
• Therefore, A* is optimal with respect to path cost; A* search never finds a sub-optimal goal

A* : The Dark Side

• A* can use lots of memory:
  $O$(number of states)
• For really big search spaces, A* will run out of memory
Devising Heuristics

Heuristics are often defined by **relaxing the problem**, i.e., computing the exact cost of a solution to a **simplified** version of problem

– remove constraints: 8-puzzle movement
– simplify problem: straight line distance for 8-puzzle and mazes

Comparing Iterative Deepening with A*  
[from Russell and Norvig, page 104, Fig 3.29]

| Depth-First Iterative Deepening (IDS) | 112 | 6,300 | $3.6 \times 10^6$ |
| A* search using "number of misplaced tiles" as the heuristic | 13 | 39 | 227 |
| A* using "Sum of Manhattan distances" as the heuristic | 12 | 25 | 73 |

Devising Heuristics

• Goal of an admissible heuristic is to get as close to the actual cost without going over

• Must also be relatively fast to compute

• Trade off:  
  use more time to compute a complex heuristic versus use more time to expand more nodes with a simpler heuristic

Devising Heuristics

• If $h(n) = h^*(n)$ for all $n$,
  – only nodes on optimal solution path are expanded
  – no unnecessary work is performed

• If $h(n) = 0$ for all $n$,
  – the heuristic is admissible
  – A* performs exactly as Uniform-Cost Search (UCS)

• The closer $h$ is to $h^*$,
  the fewer extra nodes that will be expanded
Devising Heuristics

If $h_1(n) \leq h_2(n) \leq h^*(n)$ for all $n$, then $h_2$ dominates $h_1$
- $h_2$ is a better heuristic than $h_1$
- $A^*$ using $h_1$ (i.e., $A^*_1$) expands at least as many
  if not more nodes than using $A^*$ with $h_2$ (i.e., $A^*_2$)
- $A^*_2$ is said to be better informed than $A^*_1$

Devising Heuristics

For an admissible heuristic
- $h$ is frequently very simple
- therefore search resorts to (almost) UCS
  through parts of the search space

Devising Heuristics

• If optimality is not required, i.e., satisficing solution okay, then

• Goal of heuristic is then to get as close as possible, either under or over, to the actual cost

• It results in many fewer nodes being expanded than using a poor, but provably admissible, heuristic

Devising Heuristics

$A^*$ often suffers because it cannot venture down a single path unless it is almost continuously having success (i.e., $h$ is decreasing); any failure to decrease $h$ will almost immediately cause the search to switch to another path 😞
Local Searching

- **Systematic searching:** Search for a **path** from start state to a goal state, then “execute” solution path’s sequence of operators
  - BFS, DFS, IDS, UCS, Greedy Best-First, A, A*, etc.
  - **ok** for small search spaces
  - **not okay** for NP-Hard problems requiring exponential time to find the (optimal) solution

Optimization Problems

**Now a different setting:**
- Each state \( s \) has a **score** or cost, \( f(s) \), that we can compute
- The goal is to find the state with the highest (or lowest) score, or a reasonably high (low) score
- We do **not** care about the path
- Use **variable-based models**
  - Solution is not a path but an assignment of values for a set of variables
  - **Enumerating the states is intractable**
  - Previous search algorithms are too expensive

Traveling Salesperson Problem (TSP)

- **Classic NP-Hard problem:**
  A salesperson wants to visit a list of cities
  - stopping in each city only once
  - (sometimes also must return to the first city)
  - traveling the shortest distance
  - \( f = \) total distance traveled

Traveling Salesperson Problem (TSP)

Nodes are cities
Arcs are labeled with distances between cities
Adjacency matrix (notice the graph is fully connected):

```
<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0</td>
<td>8</td>
<td>9</td>
<td>7</td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>5</td>
<td>0</td>
<td>6</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>C</td>
<td>8</td>
<td>6</td>
<td>0</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>D</td>
<td>9</td>
<td>5</td>
<td>2</td>
<td>0</td>
<td>4</td>
</tr>
<tr>
<td>E</td>
<td>7</td>
<td>5</td>
<td>3</td>
<td>4</td>
<td>0</td>
</tr>
</tbody>
</table>
```
The Traveling Salesperson Problem (TSP) is a problem in which a solution is a \( n \)-permutation of cities, called a \textit{tour}.

\begin{itemize}
  \item \textbf{How many solutions exist?}
    \begin{itemize}
      \item \( n! \) where \( n \) = \# of cities.
      \item \( n = 5 \) results in 120 tours.
      \item \( n = 10 \) results in 3,628,800 tours.
      \item \( n = 20 \) results in \( \approx 2.4 \times 10^{18} \) tours.
    \end{itemize}
\end{itemize}

\begin{itemize}
  \item \textbf{Example Problems}
    \begin{itemize}
      \item \textbf{N-Queens}
        \begin{itemize}
          \item Place \( n \) queens on \( n \times n \) checkerboard so that no queen can "capture" another.
          \item \( f = \) number of conflicting queens.
        \end{itemize}
      \item \textbf{Boolean Satisfiability}
        \begin{itemize}
          \item Given a Boolean expression containing \( n \) Boolean variables, find an assignment of \{T, F\} to each variable so that the expression evaluates to True.
          \item \( f = \) number of satisfied clauses.
        \end{itemize}
    \end{itemize}
\end{itemize}
Example Problem: Chip Layout

Lots of Chip Real Estate

Same connectivity, much less space

Example Problem: Scheduling

Also:
- parking lot layout,
- product design, aero-
- dynamic design,
- “Million Queens”
- problem, radiotherapy
- treatment planning, …

Local Searching

- Hard problems can be solved in a reasonable (i.e., polynomial) time by using either an:
  - approximate model: find an exact solution
to a simpler version of the problem
  - approximate solution: find a non-optimal solution
of the original hard problem

- We’ll explore means to search through a solution space by iteratively improving solutions until one
is found that is optimal or near optimal

Local Searching

- Local searching: every node is a solution
  - Operators/actions go from one solution to another
  - can stop at any time and have a valid solution
  - goal of search is to find a better/best solution

- No longer searching state space for a solution path and then executing the steps of the solution path

- A* isn’t a local search since it searches different partial solutions by looking at the estimated cost
  of a solution path
Local Searching

- An **operator/action** is needed to transform one solution to another
- TSP: **two-swap** operator
  - take two cities and swap their positions in the tour
  - A-B-C-D-E with swap(A,D) yields D-B-C-A-E
  - possible since graph is fully connected
- TSP: **two-interchange** operator
  - reverse the path between two cities
  - A-B-C-D-E with interchange(A,D) yields D-C-B-A-E

Neighbors: TSP

- state: A-B-C-D-E-F-G-H-A
- \( f = \) length of tour
- 2-interchange

Examples of Neighborhoods

- **N-queens**: Move queen in rightmost, most-conflicting column to a different position in that column
- **SAT**: Flip the assignment of one Boolean variable
Neighbors: SAT

- State: \((A=T, B=F, C=T, D=T, E=T)\)
- \(f\) = number of satisfied clauses
- Neighbor: flip the assignment of one variable

| \((A=T, B=F, C=F, D=T, E=T)\) | \((A=T, B=F, C=T, D=F, E=T)\) |

Local Searching

- An evaluation function, \(f\), is used to map each solution/state to a number corresponding to the quality/cost of that solution
- TSP: Use the distance of the tour path; A better solution has a shorter tour path
- Maximize \(f\): called hill-climbing (gradient ascent if continuous)
- Minimize \(f\): called or valley-finding (gradient descent if continuous)
- Can be used to maximize/minimize some cost

Hill-Climbing

- **Question**: What's a neighbor?
  - Problem spaces tend to have structure. A small change produces a neighboring state
  - The neighborhood must be small enough for efficiency
  - Designing the neighborhood is critical; This is the real ingenuity – not the decision to use hill-climbing
- **Question**: Pick which neighbor? The best one (greedy)
- **Question**: What if no neighbor is better than the current state? Stop

Hill-Climbing Algorithm

1. Pick initial state \(s\)
2. Pick \(t\) in neighbors(s) with the largest \(f(t)\)
3. if \(f(t) \geq f(s)\) then stop and return \(s\)
4. \(s = t\). Goto Step 2.

- Simple
- Greedy
- Stops at a local maximum
Hill-Climbing (HC)

- HC exploits the neighborhood
  - like Greedy Best-First search, it chooses what looks best *locally*
  - but doesn't allow backtracking or jumping to an alternative path since there is no Frontier list
- HC is very space efficient
  - Similar to Beam Search with a beam width of 1
- HC is very fast and often effective in practice

Local Optima in Hill-Climbing

- Useful mental picture: $f$ is a surface (‘hills’) in state space
  - But we can’t see the entire landscape all at once. Can only see a neighborhood; like climbing in fog.

Hill-Climbing

Visualized as a 2D surface
- Height is quality/cost of solution
  $f = f(x, y)$
- Solution space is a 2D surface
- Initial solution is a point
- Goal is to find highest point on the surface of solution space
- Hill-Climbing follows the direction of the steepest ascent, i.e., where $f$ increases the most

Solution found by HC is totally determined by the starting point; fundamental weakness is getting stuck:
- At a local maximum
- At plateaus and ridges

Global maximum may *not* be found

Trade off:
greedily exploiting locality as in HC vs. exploring state space as in BFS
Hill-Climbing with Random Restarts

- Very simple modification:
  1. When stuck, pick a random new starting state and re-run hill-climbing from there
  2. Repeat this $k$ times
  3. Return the best of the $k$ local optima

- Can be very effective
- Should be tried whenever hill-climbing is used
- Fast, easy to implement; works well for many applications where the solution space surface is not too “bumpy” (i.e., not too many local maxima)

Escaping Local Maxima

- HC gets stuck at a local maximum, limiting the quality of the solution found
- Two ways to modify HC:
  1. choice of neighborhood
  2. criterion for deciding to move to neighbor
- For example:
  1. choose neighbor randomly
  2. move to neighbor if it is better or, if it isn’t, move with some probability, $p$

Variations on Hill-Climbing

- Question: How do we make hill climbing less greedy?
  - Stochastic Hill-Climbing
    - Randomly select among the neighbors
    - The better, the more likely
    - Pros / cons compared with basic hill climbing?
  - Question: What if the neighborhood is too large to easily compute? (e.g., N-queens if we need to pick both the column and the move within it)
    - First-choice hill-climbing
      - Randomly generate neighbors, one at a time
      - If neighbor is better, take the move
      - Pros / cons compared with basic hill climbing?

Life Lesson #237

- Sometimes one needs to temporarily step backward in order to move forward
  - Lesson applied to iterative, local search:
    – Sometimes one needs to move to an inferior neighbor in order to escape a local optimum
Hill-Climbing Example: SAT

| A ∨ ¬B ∨ C | 1 |
| ¬A ∨ C ∨ D | 1 |
| B ∨ D ∨ ¬E | 0 |
| ¬C ∨ ¬D ∨ ¬E | 1 |
| ¬A ∨ ¬C ∨ E | 1 |

Maximize: \( \text{Eval(config)} = \text{# of satisfied clauses} \)

Moveset: flip any 1 variable

Example Configuration: (1,0,1,0,1)

Variations on Hill-Climbing

WALKSAT [Selman]

• Pick a random unsatisfied clause
• Select and flip a variable from that clause:
  – With prob. \( p \), pick a random variable
  – With prob. \( 1-p \), pick variable that maximizes the number of satisfied clauses
• Repeat until solution found or max number of flips attempted

This is the best known algorithm for satisfying Boolean formulas

Simulated Annealing

(Stochastic Hill-Climbing)

1. Pick initial state, \( s \)
2. Randomly pick state \( t \) from neighbors of \( s \)
3. if \( f(t) \) better than \( f(s) \)
   then \( s = t \)
   else with small probability \( s = t \)
4. Goto Step 2 until bored

Simulated Annealing

Origin:

The annealing process of heated solids – Alloys manage to find a near global minimum energy state when heated and then slowly cooled

Intuition:

By allowing occasional ascent in the search process, we might be able to escape the traps of local minima

Introduced by Nicholas Metropolis in 1953
Consequences of Occasional Bad Moves

- Helps escape local optima
- But might pass global optimum after reaching it

Idea 1: Use a small, fixed probability threshold, say, \( p = 0.1 \)

Escaping Local Optima

- Modified HC can escape from a local optimum
  - chance of making a bad move is the same at the beginning of the search as at the end
  - magnitude of improvement, or lack of, is ignored
- Fix by replacing fixed probability, \( p \), that a bad move is accepted, with a probability that decreases as the search proceeds
- Now as the search progresses, the chance of taking a bad move goes down

Control of Annealing Process

**Acceptance of a search step (Metropolis Criterion) in Hill-Climbing:**

- Let the performance change in the search be:
  \[ \Delta E = f(\text{newNode}) - f(\text{currentNode}) \]
- Always accept an ascending step (i.e., better state) \( \Delta E \geq 0 \)
- Accept a descending step only if it passes a test

Escaping Local Maxima

Let \( \Delta E = f(\text{newNode}) - f(\text{currentNode}) < 0 \)

\[ p = e^{\frac{\Delta E}{T}} \] (Boltzman's equation)

- \( \Delta E \to -\infty, \quad p \to 0 \) as badness of the move increases
  - probability of taking it decreases exponentially
- \( T \to 0, \quad p \to 0 \) as temperature decreases
  - probability of taking bad move decreases
**Probability of Moving to Worse State**

\[ x < 0 \] is region of interest

\[ e^x \]

\[ (0,1) \]

**Escaping Local Maxima**

Let \( \Delta E = f(\text{newNode}) - f(\text{currentNode}) \)

\[ p = e^{\frac{\Delta E}{T}} \] (Boltzman’s equation)

- \( \Delta E \ll T \)
  - if badness of move is small compared to \( T \), move is *likely* to be accepted
- \( \Delta E \gg T \)
  - if badness of move is large compared to \( T \), move is *unlikely* to be accepted

**Control of Annealing Process**

**Cooling Schedule:**

- \( T \), the *annealing temperature*, is the parameter that control the frequency of acceptance of bad steps
- We gradually reduce temperature \( T(k) \)
- At each temperature, search is allowed to proceed for a certain number of steps, \( L(k) \)
- The choice of parameters \( \{T(k), L(k)\} \) is called the *cooling schedule*

**Simple Cooling Schedules**

\[ T_i = T_0 - \frac{i}{N} \]

\[ T_i = T_0 \left( \frac{T_f}{T_0} \right)^{\frac{i}{N}} \]
Simulated Annealing (Stochastic Hill-Climbing)

Pick initial state, $s$
$k = 0$
while $k < k_{\text{max}}$
  $T = \text{temperature}(k)$
  Randomly pick state $t$ from neighbors of $s$
  if $f(t) > f(s)$ then $s = t$
  else if $(e^{(f(t) - f(s))/T}) > \text{random()}$ then $s = t$
  $k = k + 1$
return $s$

SA for Solving TSP

Simulated Annealing Demo

Searching for a global minimum

Simulated Annealing

- Can perform multiple backward steps in a row to escape a local optimum
- Chance of finding a global optimum increased
- Fast
  - only one neighbor generated at each iteration
  - whole neighborhood isn't checked to find best neighbor as in HC
  - Usually finds a good quality solution in a very short amount of time
Simulated Annealing

• Requires several parameters to be set
  – starting temperature
    • must be high enough to escape local optima but not too high to be random exploration of space
  – cooling schedule
    • typically exponential
  – halting temperature
• Domain knowledge helps set values:
  size of search space, bounds of maximum and minimum solutions

Simulated Annealing Issues

• Neighborhood design is critical. This is the real ingenuity – not the decision to use simulated annealing
• Evaluation function design often critical
• Annealing schedule often critical
• It’s often cheaper to evaluate an incremental change of a previously evaluated object than to evaluate from scratch. Does simulated annealing permit that?
• What if approximate evaluation is cheaper than accurate evaluation?
• Inner-loop optimization often possible

Implementation of Simulated Annealing

• This is a stochastic algorithm; the outcome may be different at different trials
• Convergence to global optimum can only be realized in an asymptotic sense
• With infinitely slow cooling rate, finds global optimum with probability 1

SA Discussion

• Simulated annealing is sometimes empirically much better at avoiding local maxima than hill-climbing. It is a successful, frequently-used, algorithm. Worth putting in your algorithmic toolbox.
• Sadly, not much opportunity to say anything formal about it (though there is a proof that with an infinitely slow cooling rate, you’ll find the global optimum)
• There are mountains of practical, and problem-specific, papers on improvements