Outline

• Advanced Search & Hill-climbing
  – More difficult problems, basics, local optima, variations

• Simulated Annealing
  – Basic algorithm, temperature, tradeoffs

• Genetic Algorithms
  – Basics of evolution, fitness, natural selection
Search vs. Optimization

Before: wanted a **path** from start state to goal state
- Uninformed search, informed search

**New setting:** optimization
- States $s$ have values $f(s)$
- Want: $s$ with optimal value $f(s)$ (i.e., optimize over states)
- Challenging setting: **too many states** for previous search approaches, but maybe not a differentiable function for SGD.
Examples: $n$ Queens

A classic puzzle:

- Place 8 queens on a 8 x 8 chessboard so that no two have the same row, column, or diagonal.
- Can generalize to $n \times n$ chessboard.

- What are states $s$? Values $f(s)$?
  - State: configuration of the board
  - $f(s)$: # of conflicting queens
Examples: TSP

Famous graph theory problem.

- Get a graph $G = (V,E)$. **Goal**: a path that visits each node exactly once and returns to the initial node (a tour).
  - State: a particular tour (i.e., ordered list of nodes)
  - $f(s)$: total weight of the tour (e.g., total miles traveled)
Examples: Satisfiability

Boolean satisfiability (e.g., 3-SAT)

- Recall our logic lecture. Conjunctive normal form

\[(A \lor \neg B \lor C) \land (\neg A \lor C \lor D) \land (B \lor D \lor \neg E) \land (\neg C \lor \neg D \lor \neg E) \land (\neg A \lor \neg C \lor E)\]

  - Goal: find if satisfactory assignment exists.
  - State: assignment to variables
  - \(f(s)\): # satisfied clauses

\[
\begin{align*}
R(x,a,d) & \land R(y,b,d) & \land R(a,b,e) & \land R(c,d,f) & \land R(z,c,0) \\
R(0,a,d) & \land R(0,b,d) & \land R(a,b,e) & \land R(c,d,1) & \land R(0,c,0) \\
R(0,a,d) & \land R(1,b,d) & \land R(a,b,e) & \land R(c,d,f) & \land R(0,c,0) \\
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R(1,a,d) & \land R(0,b,d) & \land R(a,b,e) & \land R(c,d,f) & \land R(0,c,0) \\
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\end{align*}
\]
Hill Climbing

One approach to such optimization problems.

• Basic idea: move to a neighbor with a better $f(s)$

• **Q:** how do we define **neighbor**?
  – Not as obvious as our successors in search
  – Problem-specific
  – As we’ll see, needs a careful choice
Defining Neighbors: n Queens

In n Queens, a simple possibility:

- Look at the **most-conflicting column** (ties? right-most one)
- Move queen in that column vertically to a different location
Defining Neighbors: TSP

For TSP, can do something similar:

• Define neighbors by small changes
• Example: 2-change: A-E and B-F

A-B-C-D-E-F-G-H-A

flip

A-E-D-C-B-F-G-H-A
Defining Neighbors: SAT

For Boolean satisfiability,

- Define neighbors by flipping one assignment of one variable

Starting state: TFTTT

\[(A=F, B=F, C=T, D=T, E=T)\]
\[(A=T, B=T, C=T, D=T, E=T)\]
\[(A=T, B=F, C=F, D=T, E=T)\]
\[(A=T, B=F, C=T, D=F, E=T)\]
\[(A=T, B=F, C=T, D=T, E=F)\]
\[A \lor \neg B \lor C\]
\[\neg A \lor C \lor D\]
\[B \lor D \lor \neg E\]
\[\neg C \lor \neg D \lor \neg E\]
\[\neg A \lor \neg C \lor E\]
Hill Climbing Neighbors

Q: What’s a neighbor?

- **Vague definition.** For a given problem structure, neighbors are states that can be produced by a small change.

- **Tradeoff!**
  - Too small? Will get stuck.
  - Too big? Not very efficient

- **Q:** how to pick a neighbor? Greedy

- **Q:** terminate? When no neighbor has bigger value
Hill Climbing Algorithm

Pseudocode:

1. Pick initial state \(s\)
2. Pick \(t\) in \(\text{neighbors}(s)\) with the largest \(f(t)\)
3. if \(f(t) \leq f(s)\) THEN stop, return \(s\)
4. \(s \leftarrow t\). goto 2.

What could happen? **Local optima!**
Hill Climbing: Local Optima

Q: Why is it called hill climbing?

L: What’s actually going on.

R: What we get to see.
Hill Climbing: Local Optima

Note the **local optima**. How do we handle them?
Escaping Local Optima

**Simple idea 1: random restarts**
- Stuck: pick a random new starting point, re-run.
- Do $k$ times, return best of the $k$.

**Simple idea 2: reduce greed**
- “Stochastic” hill climbing: randomly select between neighbors
- Probability proportional to the value of neighbors
Hill Climbing: Variations

Q: neighborhood too large?
• Generate random neighbors, **one at a time**. Take the better one.

Q: relax requirement to always go up?
• Often useful for harder problems
• 3SAT algorithm: Walk-SAT
Break & Quiz

Q 1.1: Hill climbing and SGD are related by
(i) Both head towards optima
(ii) Both require computing a gradient
(iii) Both will find the global optimum for a convex problem

• A. (i)
• B. (i), (ii)
• C. (i), (iii)
• D. All of the above
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Break & Quiz

Q 1.1: Hill climbing and SGD are related by

(i) Both head towards optima
(ii) Both require computing a gradient
(iii) Both will find the global optimum for a convex problem

• A. (i) (No: (iii) also true since convexity->local optima are global)
• B. (i), (ii) (No: (ii) is false. Hill-climbing looks at neighbors only.)
• C. (i), (iii)
• D. All of the above (No: (ii) false, as above.)
Simulated Annealing

A more sophisticated optimization approach.

• **Idea**: allow some downhill moves at first, then be pickier over time

• **Pseudocode:**
  
  Pick initial state $s$; $T=1$
  For $k = 0$ through $K$:
  
  $$T \leftarrow T \times 0.99 \text{ (cool down)}$$
  Pick a random neighbour $t \leftarrow \text{neighbor}(s)$
  If $f(s) \leq f(t)$, then $s \leftarrow t$
  Else with prob. $P(f(s), f(t), T)$ still do $s \leftarrow t$

  **Output**: the final state $s$
Simulated Annealing: Picking Probability

How do we pick probability $P(f(s), f(t), \text{Temp})$?

- Decrease with temperature
- Decrease with gap $f(s) - f(t)$:
  \[
  \exp\left(-\frac{|f(s) - f(t)|}{\text{Temp}}\right)
  \]

- Temperature cools over time.
  - So: high temperature, accept any $t$
  - But, low temperature, behaves like hill-climbing
  - Still, $f(s) - f(t)$ plays a role: if big, replacement probability low.
Simulated Annealing: Picking Parameters

• Have to balance the various parts., e.g., cooling schedule.
  – Too fast: becomes hill climbing, stuck in local optima
  – Too slow: takes too long.

• Combines with variations (e.g., with random restarts)
  – Probably should try hill-climbing first though.

• Inspired by cooling of metals
  – We’ll see one more alg. inspired by nature
Q 2.1: Which of the following is likely to give the best cooling schedule for simulated annealing?

A. $\text{Temp}_{t+1} = \text{Temp}_t \times 1.25$
B. $\text{Temp}_{t+1} = \text{Temp}_t$
C. $\text{Temp}_{t+1} = \text{Temp}_t \times 0.8$
D. $\text{Temp}_{t+1} = \text{Temp}_t \times 0.0001$
Q 2.1: Which of the following is likely to give the best cooling schedule for simulated annealing?

A. Temp_{t+1} = Temp_t * 1.25
B. Temp_{t+1} = Temp_t
C. Temp_{t+1} = Temp_t * 0.8
D. Temp_{t+1} = Temp_t * 0.0001
Q 2.1: Which of the following is likely to give the best cooling schedule for simulated annealing?

A. Temp_{t+1} = Temp_t * 1.25 (No, temperature is increasing)
B. Temp_{t+1} = Temp_t (No, temperature is constant)
C. Temp_{t+1} = Temp_t * 0.8
D. Temp_{t+1} = Temp_t * 0.0001 (Cools too fast---basically hill climbing)
Q 2.2: Which of the following would be better to solve with simulated annealing than A* search?

i. Finding the smallest set of vertices in a graph that involve all edges
ii. Finding the fastest way to schedule jobs with varying runtimes on machines with varying processing power
iii. Finding the fastest way through a maze

• A. (i)
• B. (ii)
• C. (i) and (ii)
• D. (ii) and (iii)
Q 2.2: Which of the following would be better to solve with simulated annealing than A* search?

i. Finding the smallest set of vertices in a graph that involve all edges

ii. Finding the fastest way to schedule jobs with varying runtimes on machines with varying processing power

iii. Finding the fastest way through a maze

• A. (i)
• B. (ii)
• C. (i) and (ii)
• D. (ii) and (iii)
Q 2.2: Which of the following would be better to solve with simulated annealing than A* search?

i. Finding the smallest set of vertices in a complete graph (i.e., all nodes connected)
ii. Finding the fastest way to schedule jobs with varying runtimes on machines with varying processing power
iii. Finding the fastest way through a maze

• A. (i) (No, (ii) better: huge number of states, don’t care about path)
• B. (ii) (No, (i) complete graph might have too many edges for A*)
• C. (i) and (ii)
• D. (ii) and (iii) (No, (iii) is good for A*: few successors, want path)
Genetic Algorithms

Another optimization approach based on nature

- Survival of the fittest!
Evolution Review

Encode genetic information in DNA (four bases)
• A/C/T/G: nucleobases acting as symbols

• Two types of changes
  – Crossover: exchange between parents’ codes
  – Mutation: rarer random process
    • Happens at individual level
Natural Selection

Competition for resources

• Organisms better fit $\Rightarrow$ better probability of reproducing
• Repeated process: fit become larger proportion of population

Goal: use these principles for optimization

– New terminology: state $s$ ‘individual’
– Value $f(s)$ is now the ‘fitness’
Genetic Algorithms Setup I

Keep around a fixed number of states/individuals

• A bit like beam search
• Call this the **population**

For our n Queens game example, an individual:

(3 2 7 5 2 4 1 1)
Goal of genetic algorithms: optimize using principles inspired by mechanism for evolution

- E.g., analogous to **natural selection, cross-over, and mutation**

![Diagram of genetic algorithm process]

- Initial Population
- Fitness Function
- Selection
- Cross-Over
- Mutation

# of non-attacking pairs

prob. reproduction \( \propto \) fitness

\[24748552 \rightarrow 32752411 \rightarrow 32748552 \rightarrow 32748\underline{152} \]

\[32752411 \rightarrow 24748552 \rightarrow 24752411 \rightarrow 24752411 \]

\[24415124 \rightarrow 32752411 \rightarrow 32752124 \rightarrow 32252124 \]

\[32543213 \rightarrow 24415124 \rightarrow 24415411 \rightarrow 2441541\underline{7} \]
Genetic Algorithms Pseudocode

Just one variant:

1. Let $s_1, \ldots, s_N$ be the current population
2. Let $p_i = f(s_i) / \sum_j f(s_j)$ be the reproduction probability
3. for $k = 1; k < N; k+=2$
   • parent1 = sample with replacement according to $p$
   • parent2 = sample with replacement according to $p$
   • randomly select a crossover point, swap strings of parents 1, 2 to generate children $t[k], t[k+1]$
4. for $k = 1; k <= N; k++$
   • Randomly mutate each position in $t[k]$ with a small probability (mutation rate)
5. The new generation replaces the old: \{ $s$ \} $\leftarrow$ \{ $t$ \}. Repeat
Reproduction: Proportional Selection

Reproduction probability: $p_i = \frac{f(s_i)}{\sum_j f(s_j)}$

- **Example**: $\sum_j f(s_j) = 5+20+11+8+6=50$
- $p_1=5/50=10\%$

<table>
<thead>
<tr>
<th>Individual</th>
<th>Fitness</th>
<th>Prob.</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>5</td>
<td>10%</td>
</tr>
<tr>
<td>B</td>
<td>20</td>
<td>40%</td>
</tr>
<tr>
<td>C</td>
<td>11</td>
<td>22%</td>
</tr>
<tr>
<td>D</td>
<td>8</td>
<td>16%</td>
</tr>
<tr>
<td>E</td>
<td>6</td>
<td>12%</td>
</tr>
</tbody>
</table>
Example: Scheduling Courses

Let’s run through an example:

- 5 courses: A, B, C, D, E
- 3 time slots: Mon/Wed, Tue/Thu, Fri/Sat
- Students wish to enroll in three courses
- Goal: maximize student enrollment

<table>
<thead>
<tr>
<th>Courses</th>
<th>Students</th>
</tr>
</thead>
<tbody>
<tr>
<td>A B C</td>
<td>2</td>
</tr>
<tr>
<td>A B D</td>
<td>7</td>
</tr>
<tr>
<td>A D E</td>
<td>3</td>
</tr>
<tr>
<td>B C D</td>
<td>4</td>
</tr>
<tr>
<td>B D E</td>
<td>10</td>
</tr>
<tr>
<td>C D E</td>
<td>5</td>
</tr>
</tbody>
</table>
Example: Scheduling Courses

Let’s run through an example:

• State: course assignment to time slot

<table>
<thead>
<tr>
<th>M</th>
<th>M</th>
<th>F</th>
<th>T</th>
<th>M</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>B</td>
<td>C</td>
<td>D</td>
<td>E</td>
</tr>
</tbody>
</table>

= MMFTM

• Here:
  – Courses A, B, E scheduled Mon/Wed
  – Course D scheduled Tue/Thu
  – Course C scheduled Fri/Sat

<table>
<thead>
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<tr>
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Example: Scheduling Courses

Value of a state? Say MMFTM

<table>
<thead>
<tr>
<th>Courses</th>
<th>Students</th>
<th>Can enroll?</th>
</tr>
</thead>
<tbody>
<tr>
<td>A B C</td>
<td>2</td>
<td>No</td>
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<tr>
<td>B D E</td>
<td>10</td>
<td>No</td>
</tr>
<tr>
<td>C D E</td>
<td>5</td>
<td>Yes</td>
</tr>
</tbody>
</table>

- Here 4+5=9 students can enroll in desired courses
Example: Scheduling Courses

First step:
• Randomly initialize and evaluate states

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<tr>
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<td>10</td>
</tr>
<tr>
<td>C D E</td>
<td>5</td>
</tr>
</tbody>
</table>

- MMFTM = 9  MMFTM = 26%
- TTFMM = 4  TTFMM = 11%
- FMTTF = 19 FMTTF = 54%
- MTTTF = 3  MTTTF = 9%

• Calculate reproduction probabilities
Example: Scheduling Courses

Next steps:

• Select parents using reproduction probabilities
• Perform crossover
• Randomly mutate new children

```plaintext
MMFTM = 26%  
TTFMM = 11%  
FMTTF = 54%  
MTTTF = 9%  

FMTTF  
MMFTM  
FMTTF  

FMTTF  
MMFTM  
FMTTF  

FMTTF  
MMFTM  
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MMFTM  
FMTTF  
```
Example: Scheduling Courses

Continue:

• Now, get our function values for updated population
• Calculate reproduction probabilities

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<td>10</td>
</tr>
<tr>
<td>C D E</td>
<td>5</td>
</tr>
</tbody>
</table>

\[
\begin{align*}
FMFTT & = 11 & FMFTT & = 39\% \\
MMTTF & = 13 & MMTTF & = 46\% \\
MMTFF & = 4  & MMTFF & = 14\% \\
FTTTF & = 0  & FTTTF & = 0\% \\
\end{align*}
\]
Variations & Concerns

Many **possibilities:**
- Parents survive to next generation
- Use ranking instead of exact value of $f(s)$ for reproduction probabilities (reduce influence of extreme f values)

Some **challenges**
- State encoding
- Lack of diversity: converge too soon
- Must pick a lot of parameters
Summary

• Challenging optimization problems
  – First, try hill climbing. Simplest solution

• Simulated annealing
  – More sophisticated approach; helps with local optima

• Genetic algorithms
  – Biology-inspired optimization routine