

# CS 540 Introduction to Artificial Intelligence Search III: Advanced Search (aka Optimization)

University of Wisconsin-Madison Fall 2025 Sections 1 & 2

#### **Announcements**

- Homework:
  - HW9 due today at 11:59 PM
  - HW10 released today, due Tuesday December 9
- Final Exam:
  - December 13 12:25 2:25 PM
  - Location for sections 001 AND 002 (Instructor Blerina Gkotse)
    - Chemistry S413 (Last name starting with A-J inclusive)
    - Engineering Hall 1800 (Last name starting with K-Sa inclusive)
    - Van Vleck B130 (Last name starting with Sc-Z inclusive)
  - Students with McBurney accommodations or alternate requests will be notified about the exam time and location.
- Course evaluation

Class roadmap: Ethics and Trust in AI

Review

#### **Advanced Search Overview**

**Problem Setting** 

How is a search problem defined?

How different from other search types?

Hill Climbing

Neighbors Local vs. global optima Genetic Algorithms

What is difference between two?

Fitness
Population
Cross-over
Mutation

#### **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

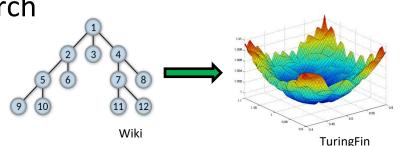
# Search vs. Optimization

Before: wanted a path from start state to goal state

Uninformed search, informed search

**New setting**: optimization

- States s have values f(s)
- Want: Find s with optimal value f(s) (i.e, optimize over states)
- Challenging settings: too many states for previous search approaches, but maybe not a differentiable function for gradient descent.



### Examples: n Queens

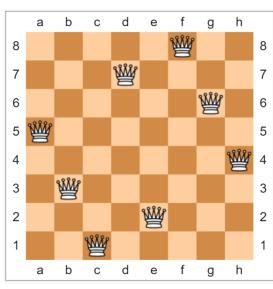
#### A classic puzzle:

Place 8 queens on 8 x 8 chessboard so that no two have same

row, column, or diagonal.

Can generalize to n x n chessboard.

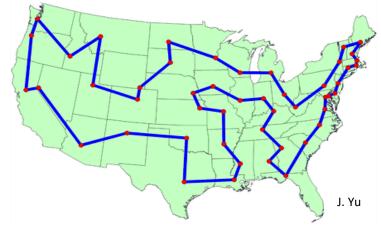
- What are states s? Values f(s)?
  - State: configuration of the board
  - f(s): # of non-conflicting queens



### **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**

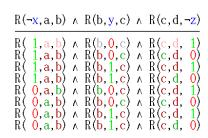
#### Boolean satisfiability (e.g., 3-SAT)

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

R(x,a,d)	٨	R(y,b,d)	٨	R(a,b,e)	٨	R(c,d,f)	٨	R(z,c,0)
R(0,a,d) R(0,a,d) R(0,a,d) R(0,a,d) R(1,a,d) R(1,a,d) R(1,a,d) R(1,a,d)	>>>>>>>	R(0,b,d) R(0,b,d) R(1,b,d) R(1,b,d) R(0,b,d) R(0,b,d) R(1,b,d) R(1,b,d)	> > > > > > >	R(a,b,e) R(a,b,e) R(a,b,e) R(a,b,e) R(a,b,e) R(a,b,e) R(a,b,e) R(a,b,e)	>>>>>>>>	R(c,d,f) R(c,d,f) R(c,d,f) R(c,d,f) R(c,d,f) R(c,d,f) R(c,d,f) R(c,d,f) R(c,d,f)	>>>>>>>>	R(0,c,0) R(1,c,0) R(0,c,0) R(1,c,0) R(0,c,0) R(1,c,0) R(0,c,0) R(1,c,0)



# Hill Climbing

#### One approach to such optimization problems

Basic idea: start at one state, move to a neighbor with a better f(s) value, repeat until no neighbors have better f(s) value.

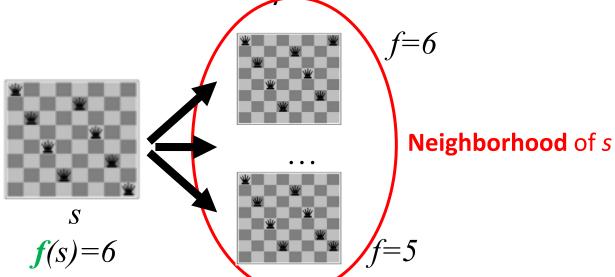
- Q: how do we define neighbor?
  - Not as obvious as our successors in search
  - Problem-specific
  - As we'll see, needs a careful choice



### Defining Neighbors: n Queens

#### In n Queens, a simple possibility:

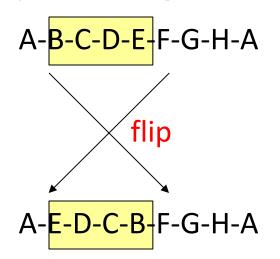
- Look at the most-conflicting column (ties? right-most one)
- Move queen in that column vertically to a different location

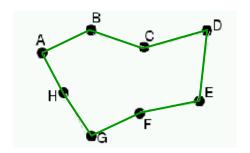


# Defining Neighbors: TSP

#### For TSP, can do something similar:

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





# **Defining Neighbors: SAT**

#### For Boolean satisfiability,

Define neighbors by flipping one assignment of one variable
 Starting state: (A=T, B=F, C=T, D=T, F=T)

### 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!

- Neighborhood too small? Will get stuck.
- Neighborhood too big? Not very efficient
- Q: how to pick a neighbor? Greedy
- Q: terminate? When no neighbor has better value

### Hill Climbing Algorithm

#### **Pseudocode:**

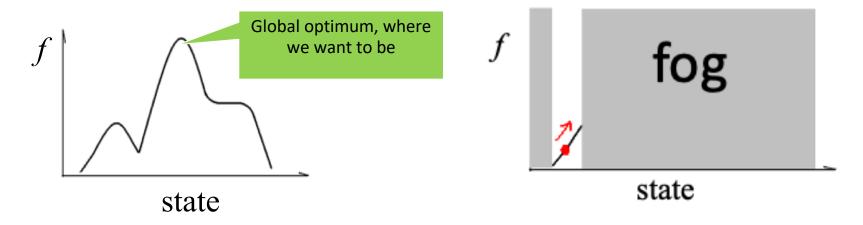
- 1. Pick initial state s
- 2. Pick t in **neighbors**(s) with the best f(t)
- 3. if f(t) is not better than f(s) THEN stop, return s
- 4.  $s \leftarrow t$ . goto 2.



What could happen? Local optima!

### Hill Climbing: Local Optima

**Q**: Why is it called hill climbing?

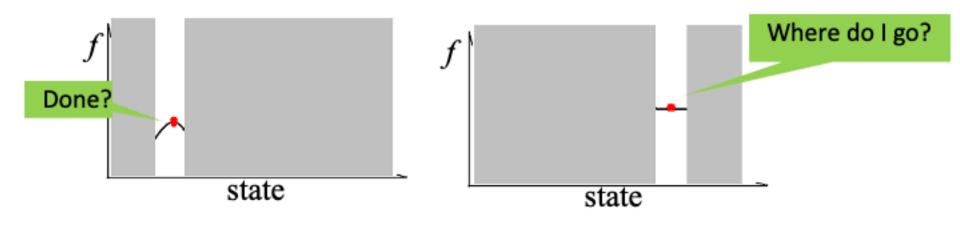


L: What's actually going on.

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 runs.

#### Simple idea 2: reduce greed

- "Stochastic" hill climbing: randomly select between neighbors.
- Probability of selecting a neighbor should be proportional to the value of that neighbor.

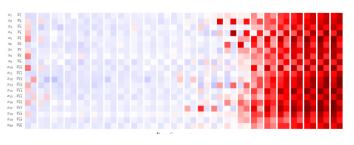
### Hill Climbing: Variations

**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



- **Q 1.1**: Hill climbing and stochastic gradient descent 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 (problem where all optima have the same value).
- A. (i)
- B. (i), (ii)
- C. (i), (iii)
- D. All of the above

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- A. (i)
- B. (i), (ii) (No: (ii) is false. Hill-climbing looks at neighbors only.)
- C. (i), (iii)
- D. All of the 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:

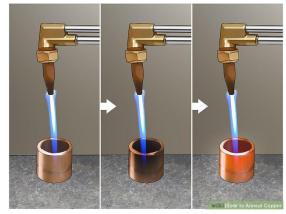
T \leftarrow T^*0.99 \ (cool\ down)

Pick a random neighbour t \leftarrow neighbor(s)

If f(t) better than f(s), then s \leftarrow t

Else with prob. P(f(s), f(t), T) still do s \leftarrow t

Output: the best state ever seen
```



wikihow.com

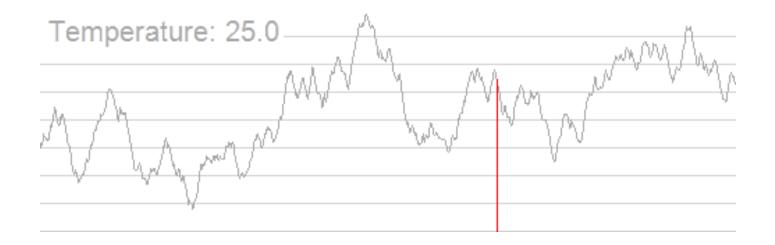
# Simulated Annealing: Picking Probability

How do we pick probability P? Note 3 parameters.

- Decrease with time
- Decrease with gap |f(s) f(t)|:  $\exp\left(-\frac{|f(s) f(t)|}{Temp}\right)$
- 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: Visualization

What does it look like in practice?



### 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.  $Temp_{t+1} = Temp_t * 1.25$
- B.  $Temp_{t+1} = Temp_t$
- C.  $Temp_{t+1} = Temp_t * 0.8$
- D.  $Temp_{t+1} = Temp_t * 0.0001$

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- 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, temperate 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 hill climbing rather than A\* search?

- 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)

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**Q 2.2**: Which of the following would be better to solve with hill climbing rather than A\* search?

- 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) (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

#### Optimization approach based on nature

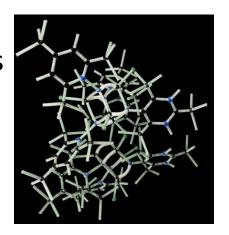
Survival of the fittest!

#### **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 with better fitness → better probability of reproducing
- Repeated process: fit become larger proportion of population

#### Goal: use these principles for optimization

- New terminology: state is 'individual'
- Value f(s) is now the 'fitness'

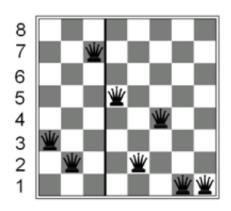


### Genetic Algorithms Setup I

Keep around a fixed number of states/individuals

Call this the population

For our n Queens game example, an individual:



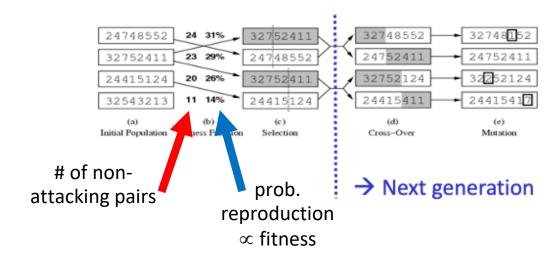
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# Genetic Algorithms Setup II

Goal of genetic algorithms: optimize using principles inspired by mechanism for evolution

Analogous to natural selection, cross-over, and mutation



### Genetic Algorithms Pseudocode

#### Just one variant:

- 1. Let  $s_1, ..., s_N$  be the current population
- 2. Let  $p_i = f(s_i) / \sum_i f(s_i)$  be the reproduction probability
- 3. for k = 1; k < N; k + = 2
  - parent1 = randomly pick according to p
  - parent2 = randomly pick another
  - 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:  $p_i = f(s_i) / \Sigma_j f(s_j)$ 

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

Individual	Fitness	Prob.
Α	5	10%
В	20	40%
С	11	22%
D	8	16%
E	6	12%



#### 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

Courses	Students
АВС	2
ABD	7
ADE	3
BCD	4
BDE	10
CDE	5

#### Let's run through an example:

State: course assignment to time slot

М	М	F	Т	М
Α	В	С	D	Е

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

Courses	Students
АВС	2
ABD	7
ADE	3
BCD	4
BDE	10
CDE	5

Value of a state? Say MMFTM

Courses	Students	Can enroll?
АВС	2	No
ABD	7	No
ADE	3	No
BCD	4	Yes
BDE	10	No
CDE	5	Yes

Here 4+5=9 students can enroll in desired courses

#### First step:

Randomly initialize and evaluate states

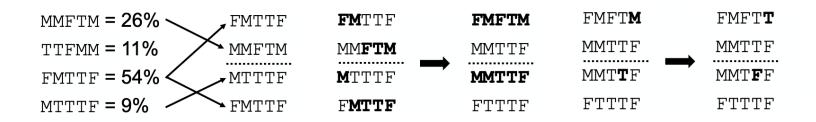
MMFTM = 9	MMFTM = 26%
TTFMM = 4	TTFMM = 11%
FMTTF = 19	FMTTF = <b>54</b> %
MTTTF = 3	MTTTF = <b>9</b> %

Calculate reproduction probabilities

Courses	Students
АВС	2
ABD	7
ADE	3
BCD	4
BDE	10
CDE	5

#### Next steps:

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



#### Continue:

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

FMFTT = 11	FMFTT = <b>39</b> %
MMTTF = 13	MMTTF = <b>46</b> %
MMTFF = 4	MMTFF = <b>14%</b>
FTTTF = 0	FTTTF = 0%

Courses	Students
АВС	2
ABD	7
ADE	3
BCD	4
BDE	10
CDE	5

#### **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

- Formulating a good 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

### **Suggested Readings**

Textbook: Artificial Intelligence: A Modern Approach (4th edition). Stuart Russell and Peter Norvig. Pearson, 2020.

Chapter 4