CS 540 Introduction to Artificial Intelligence
Search III: Advanced Search

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Announcements

- **Homeworks**:
  - HW8 due Tuesday.

- **Class roadmap:**
  - Today: Search III
  - Tuesday before and after Thanksgiving: Game (uses Search)

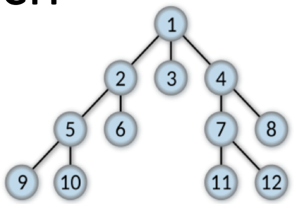
Outline

- 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



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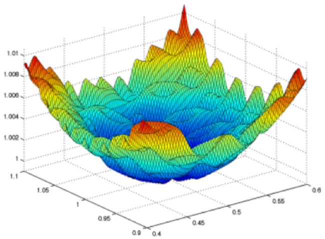

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New setting: optimization

- 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 continuous function for SGD.

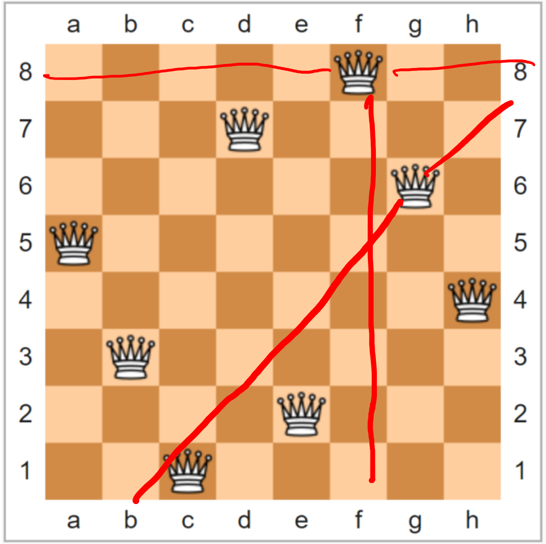
$$f(s) = \begin{cases} 0 & \text{if no conflict} \\ 1 & \text{if there's conflict.} \end{cases}$$

Examples: *n* Queens

A classic puzzle:

- Place 8 queens on a 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 conflicting queens



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Examples: TSP

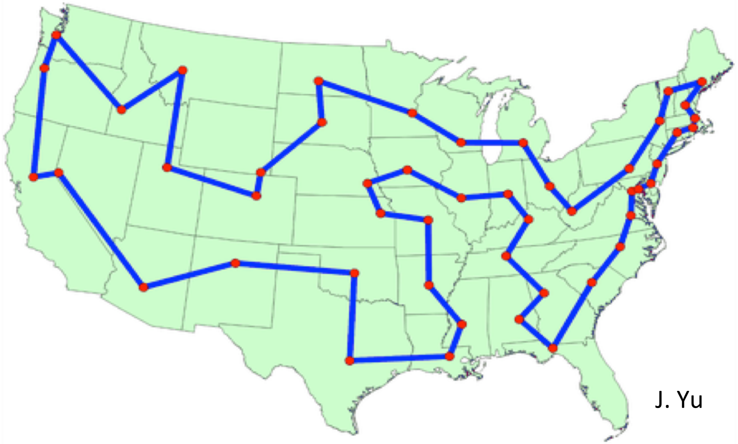
Traveling Salesman Problem

Famous graph theory problem.

optionally: find shortest tour.

- 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)



J. Yu

Examples: Satisfiability

AND AND.

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

- Recall our logic lecture. Conjunctive normal form

$$\underbrace{(A \vee \neg B \vee C)}_{\text{clause}} \wedge (\neg A \vee C \vee D) \wedge (B \vee D \vee \neg E) \wedge (\neg C \vee \neg D \vee \neg E) \wedge (\neg A \vee \neg C \vee E)$$

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

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

R(¬x,a,b)	∧	R(b,y,c)	∧	R(c,d,¬z)
R(1,a,b)	∧	R(b,0,c)	∧	R(c,d, 1)
R(1,a,b)	∧	R(b,0,c)	∧	R(c,d, 0)
R(1,a,b)	∧	R(b,1,c)	∧	R(c,d, 1)
R(1,a,b)	∧	R(b,1,c)	∧	R(c,d, 0)
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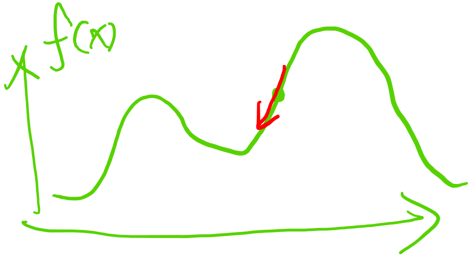
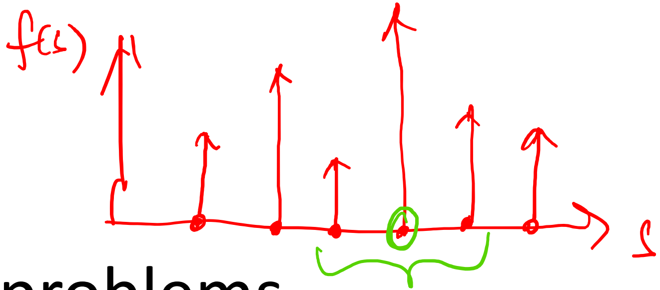


Hill Climbing



One approach to such optimization problems.

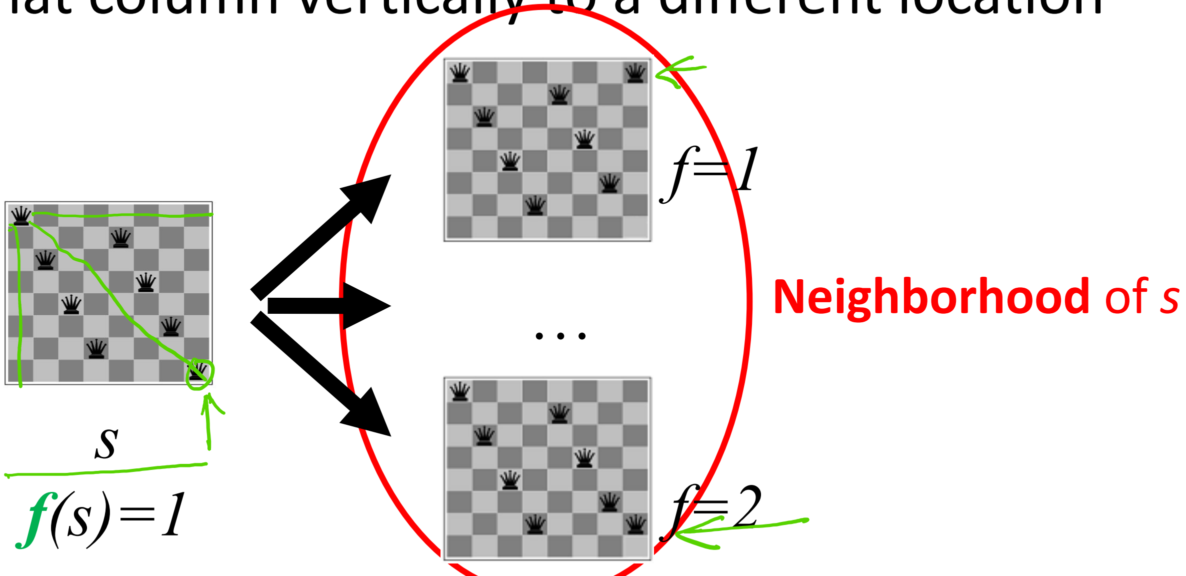
- Basic idea: move to a neighbor with a better ***f***(*s*)

- **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:

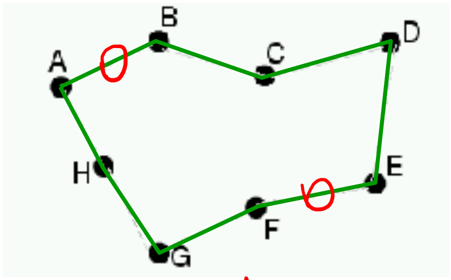
- Define neighbors by small changes
- Example: 2-change: A-E and B-F

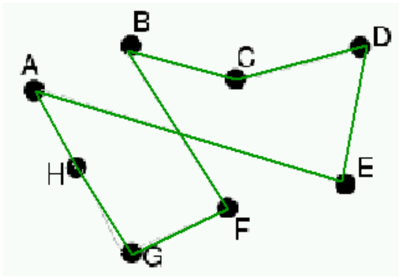
A-$\boxed{\text{B-C-D-E}}$-F-G-H-A

flip

A-$\boxed{\text{E-D-C-B}}$-F-G-H-A

S





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 struck.
  - Too big? Not very efficient

- **Q**: how to pick a neighbor? Greedy
- **Q**: terminate? When no neighbor has bigger value

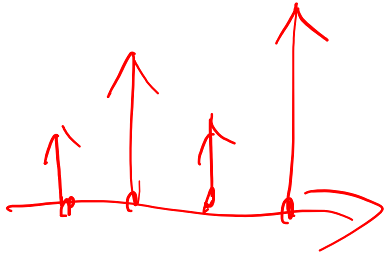
Hill Climbing Algorithm

max f

Pseudocode:

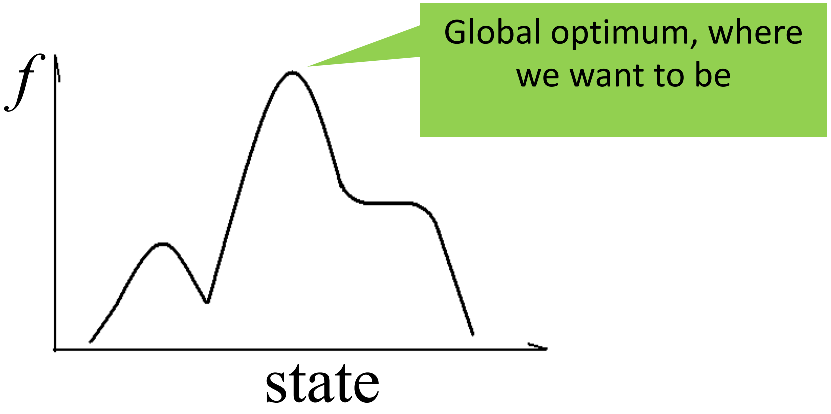
1. Pick initial state *s*
2. Pick *t* in **neighbors**(*s*) with the largest $f(t)$
3. if $f(t) \leq f(s)$ THEN stop, return *s*
4. $s \leftarrow t$. goto 2.

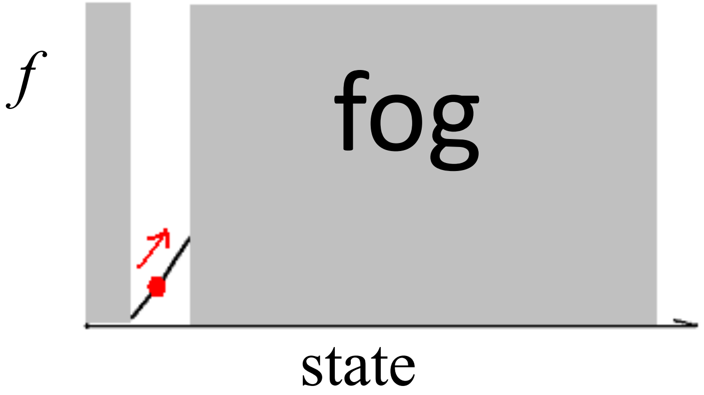
What could happen? **Local optima!**



Hill Climbing: Local Optima

Q: Why is it called hill climbing?



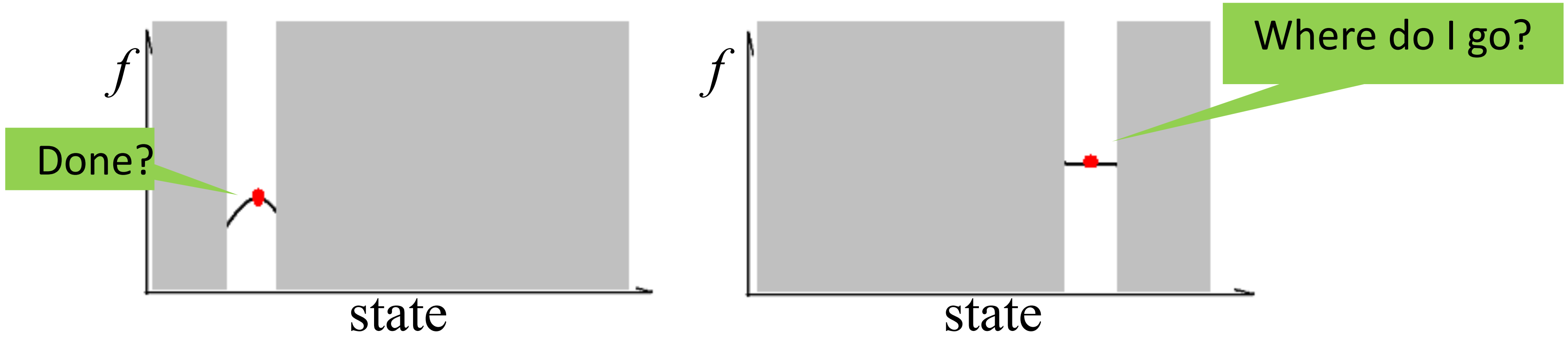


L: What's actually going on.

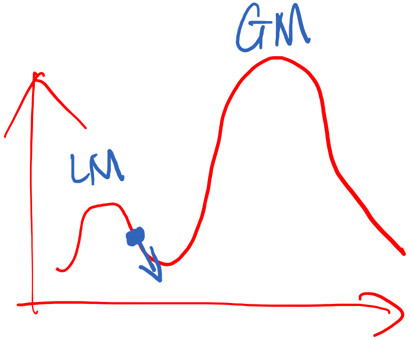
R: What we get to see.

Hill Climbing: Local Optima

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



Escaping Local Optima

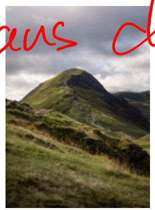


Simple idea 1: random restarts

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

Similar to k-means clustering





Simple idea 2: reduce greed

- "Stochastic" hill climbing: randomly select between neighbors
- Probability proportional to the value of neighbors

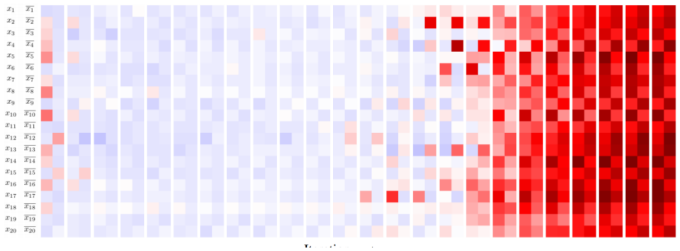
Hill Climbing: Variations

Q: neighborhood too large?

- Generate a few 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



D. Selsam

Break & Quiz

Q 1.1: Hill climbing and SGD are related by

(i) Both head towards local optima

(ii) Both require computing a gradient

(iii) Both will find the global optimum for a convex problem (when minimizing)

- A. (i)
- B. (i), (ii)
- C. (i), (iii)
- D. All of the above

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Q 1.1: Hill climbing and SGD are related by

(i) Both head towards local optima

(ii) Both require computing a gradient

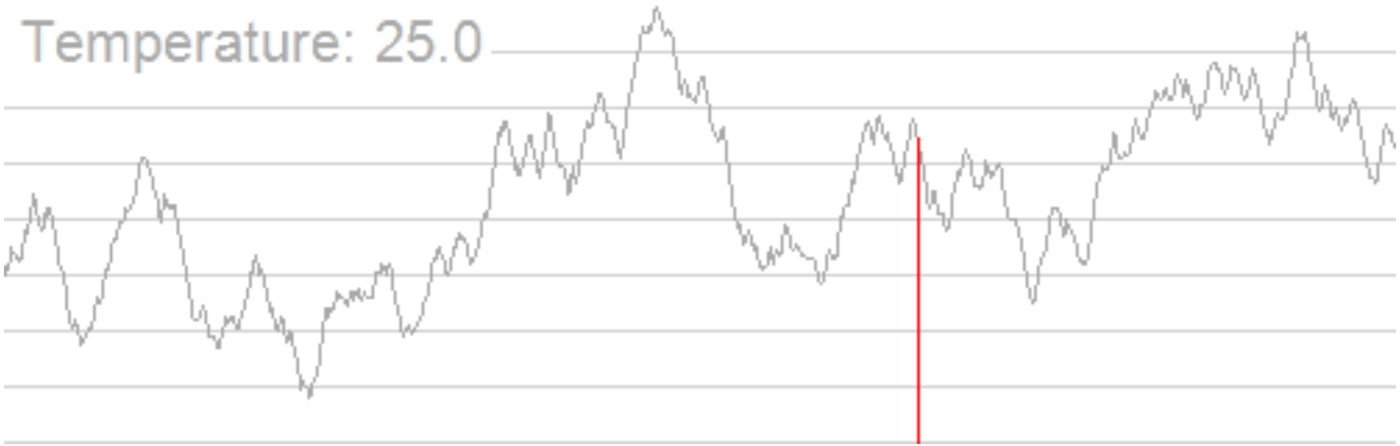
(iii) Both will find the global optimum for a convex problem (when minimizing)

- 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**: move quickly at first, then slow down



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Simulated Annealing

A more sophisticated optimization approach.

- **Idea**: move quickly at first, then slow down
- Pseudocode:

Pick initial state x
For k = 0 through k_{max}:
    Reduce temperature $\boldsymbol{T}$
    Pick a random neighbour, $y \leftarrow$ neighbor(x)
    If f(y) $\geq f(x)$, then $x \leftarrow y$
    Else, with prob. $P(f(x), f(y), \boldsymbol{T})$ then $x \leftarrow y$
Output: the final state x

The interesting bit

Simulated Annealing: Picking Probability

How do we pick probability P?

- Decrease with gap $|f(x) - f(y)|$
- Decrease with time k

Pick initial state x
For k = 0 through k_{max}:
    Reduce temperature T
    Pick a random neighbour, $y \leftarrow$ neighbor(x)
    If $f(y) \geq f(x)$, then $x \leftarrow y$
    Else, with prob. $P(f(x), f(y), T)$ then $x \leftarrow y$
Output: the final state x

Simulated Annealing: Picking Probability

temperature

How do we pick probability *P*?

$$P(x, y, \boldsymbol{T}) = \exp\left(-\frac{|f(x) - f(y)|}{\boldsymbol{T}}\right)$$

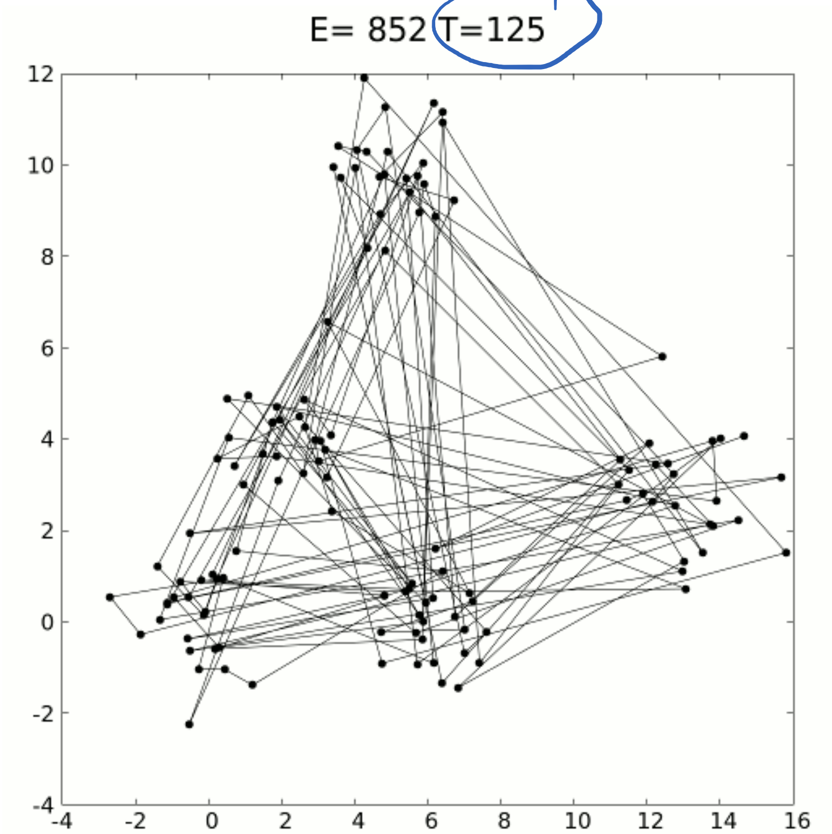
- Decrease with gap $|\boldsymbol{f}(x) - \boldsymbol{f}(y)|$
- Decrease with time *k*

large T $= \exp\left(-\frac{?}{10000}\right) \approx \exp(-0) \approx 1$

small T $= \exp\left(-\frac{?}{0.001}\right) \approx \exp(-\text{large}) \approx 0.$

- Temperature ***T*** cools over time
  - High temperature, accept any *y*
  - Low temperature, behaves like hill-climbing
  - Still, $|\boldsymbol{f}(x) - \boldsymbol{f}(y)|$ plays a role: if big, replacement probability low.

Simulated Annealing: Visualization



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Simulated Annealing: Picking Parameters

how to reduce T.

- 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

Break & Quiz

Q 2.1: Which of the following is likely to give the best cooling schedule for simulated annealing?

k = iteration count

A. $Temp_{k+1} = Temp_k * 1.25$

B. $Temp_{k+1} = Temp_k$

C. $Temp_{k+1} = Temp_k * 0.8$

D. $Temp_{k+1} = Temp_k * 0.0001$

Break & Quiz

Q 2.1: Which of the following is likely to give the best cooling schedule for simulated annealing?

A. $Temp_{k+1}$= $Temp_k$* 1.25
B. $Temp_{k+1}$= $Temp_k$
C. $Temp_{k+1}$= $Temp_k$* 0.8
D. $Temp_{k+1}$= $Temp_k$* 0.0001

$$Temp_{k+1} = \frac{1}{k+1}$$

Break & Quiz

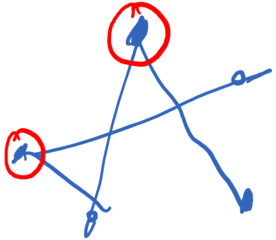
Q 2.1: Which of the following is likely to give the best cooling schedule for simulated annealing?

A. $Temp_{k+1} = Temp_k * 1.25$ (No, temperate is increasing)

B. $Temp_{k+1} = Temp_k$ (No, temperature is constant)

C. $Temp_{k+1} = Temp_k * 0.8$

D. $Temp_{k+1} = Temp_k * 0.0001$ (Cools too fast---basically hill climbing)



Break & Quiz

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)

Break & Quiz

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- **C. (i) and (ii)**
- D. (ii) and (iii)

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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) (Too many states for A*, don't care about path)
- B. (ii) (Similar to above)
- **C. (i) and (ii)**
- D. (ii) and (iii) ((iii) is good for A*: few successors, want path)

Genetic Algorithms

Another optimization approach based on nature

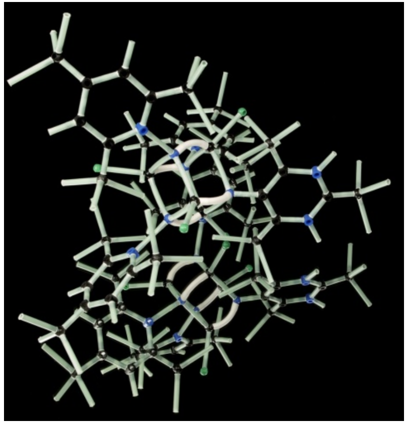
- Survival of the fittest!

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



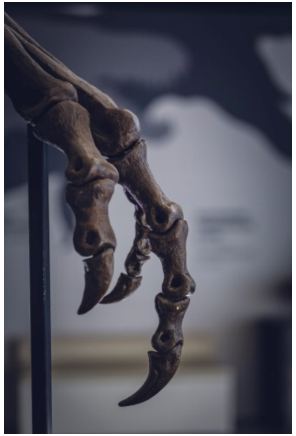
Natural Selection

Competition for resources

- Organisms better fit ➔ 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**’

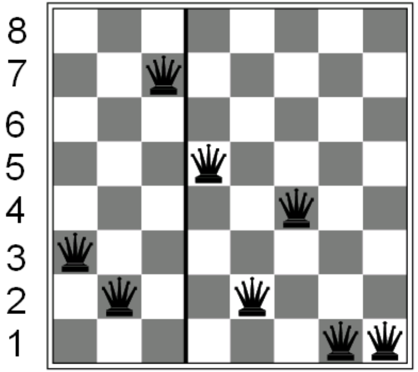


Genetic Algorithms Setup I

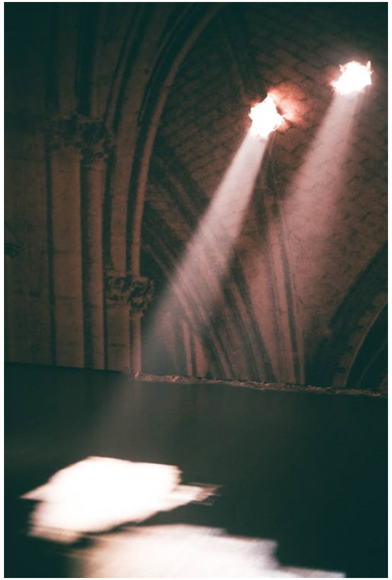
Keep around a fixed number of states/individuals

- 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)

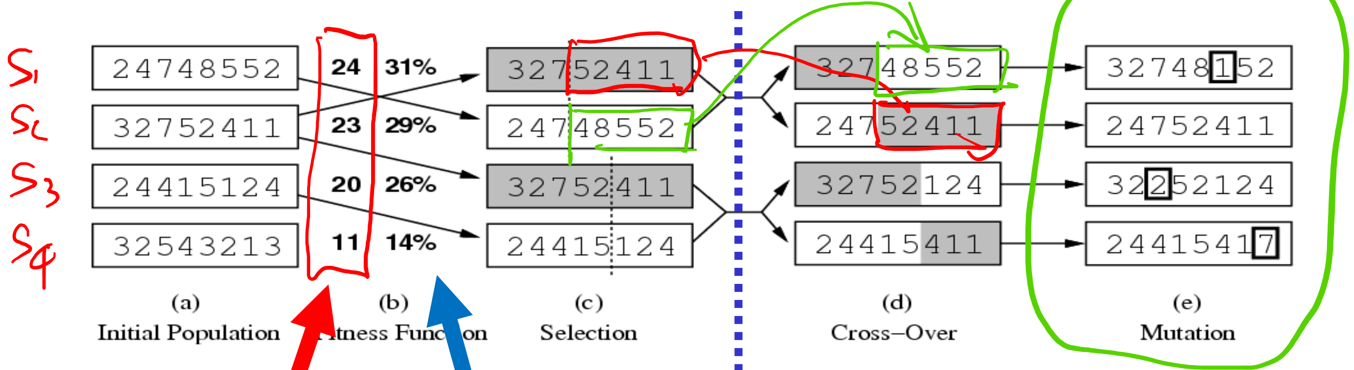


$\frac{8\times7}{2} = 28$

Genetic Algorithms Setup II

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

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



$f(s) =$ # of non-attacking pairs

prob. reproduction ∝ fitness

→ Next generation

Genetic Algorithms Pseudocode

Just one variant:

1. Let $s_1, \ldots, s_N$ be the current population
2. Let $p_i = \boldsymbol{f}(s_i) / \Sigma_j \boldsymbol{f}(s_j)$ 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: $p_i = \boldsymbol{f}(s_i)\ /\ \Sigma_j\, \boldsymbol{f}(s_j)$

- **Example**: $\Sigma_j\, \boldsymbol{f}(s_j) = 5+20+11+8+6=50$
- p_1=5/50=10%

s $\qquad$ $f(s)$

Individual	Fitness	Prob.	
A	5	10%	= 5/50
B	20	40%	= 20/50
C	11	22%	= 11/50
D	8	16%	= 8/50
E	6	12%	= 6/50

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

Courses	Students
A B C	2
A B D	7
A D E	3
B C D	4
B D E	10
C D E	5

Example: Scheduling Courses

Let's run through an example:

- State: course assignment to time slot

M	M	F	T	M
A	B	C	D	E

= MMFTM

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

Courses	Students
A B C	2
A B D	7
A D E	3
B C D	4
B D E	10
C D E	5

Example: Scheduling Courses

Value of a state? Say MMFTM

Courses	Students	Can enroll?
A B C	2	No
A B D	7	No
A D E	3	No
B C D	4	Yes
B D E	10	No
C D E	5	Yes

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

Example: Scheduling Courses

First step:

- Randomly initialize and evaluate states

S_1	MMFTM = 9	S_1'	8	MMFTM = 26%	$= \frac{9}{9+4+19+3}$
S_2	TTFMM = 4	S_2'	3	TTFMM = 11%	
S_3	FMTTF = 19	S_3'	11	FMTTF = 54%	
S_4	MTTTF = 3	S_4'	2	MTTTF = 9%	

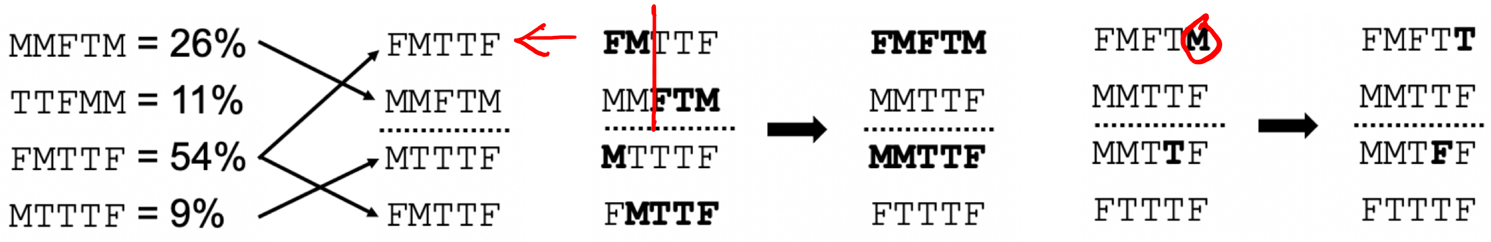
- Calculate reproduction probabilities

Courses	Students
A B C	2
A B D	7
A D E	3
B C D	4
B D E	10
C D E	5

Example: Scheduling Courses

Next steps:

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



Example: Scheduling Courses

Continue:

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

`FMFTT` = 11	`FMFTT` = 39%
`MMTTF` = 13	`MMTTF` = 46%
`MMTFF` = 4	`MMTFF` = 14%
`FTTTF` = 0	`FTTTF` = 0%

Courses	Students
A B C	2
A B D	7
A D E	3
B C D	4
B D E	10
C D E	5

Variations & Concerns

Many **possibilities**:

- Parents survive to next generation
- Ranking instead of exact value of $\boldsymbol{f}(s)$ for reproduction probabilities

Some **challenges**

- State encoding
- Lack of diversity: converge too soon
- Must pick a lot of parameters

Global optimization.

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

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