CS 540 Introduction to Artificial Intelligence

Search III: Advanced Search (aka Optimization)

University of Wisconsin-Madison

Spring 2025

Announcements

- **Homework**:
  - HW10 due on **Wednesday April 30th at 11:59 PM**
- **Final Exam:**
  - **May 7th 07:45 - 09:45 AM**
  - **Lecture 001 (MW 14:30 - 15:45): S429 Chemistry Building**
  - **Lecture 002 (TR 11:00 - 12:15): 1220 Microbial Sciences**
  - **Lecture 003 (TR 16:00 - 17:15): B10 Ingraham Hall**
  - Students with Mc Burney accommodations or alternate requests will be notified about the exam time and location.
- **Course evaluation**
- Class roadmap:

Advanced Search
Ethics and Trust in AI

Advanced Search Overview

Problem Setting

How is a search problem defined?

How different from other search types?

Hill Climbing

Genetic Algorithms

What is difference between two?

Neighbors
Local vs. global optima

Fitness
Population
Cross-over
Mutation

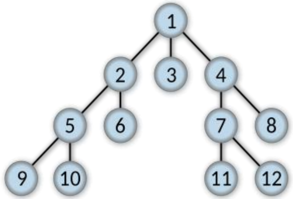
Outline

- 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



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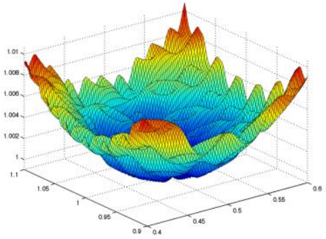
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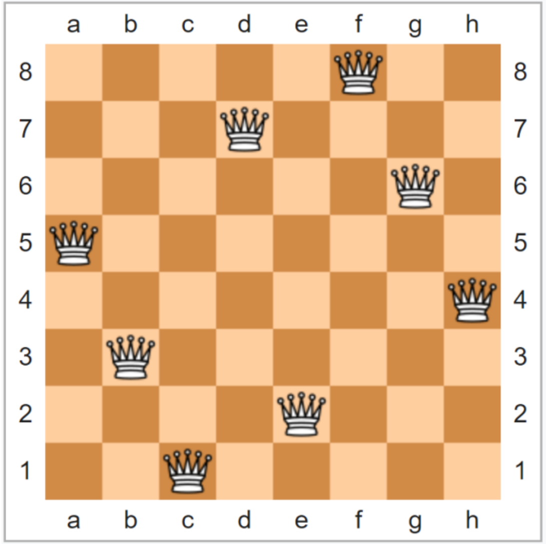
New setting: optimization

- 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.



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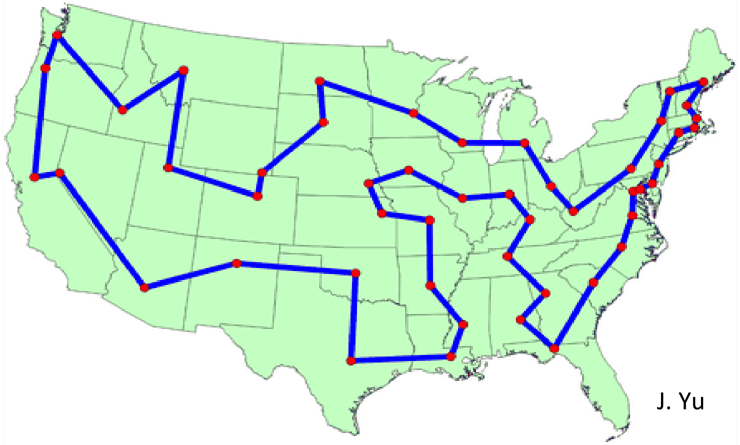
- What are states *s*? Values ***f***(*s*)?
  - State: configuration of the board
  - ***f***(*s*): # of non-conflicting queens

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)



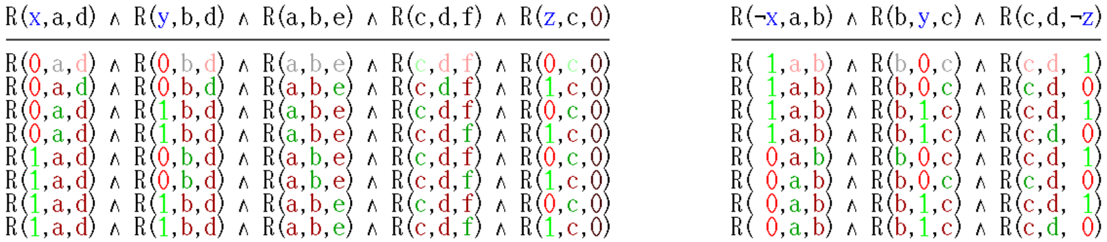
Examples: Satisfiability

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

- Recall our logic lecture. Conjunctive normal form

$(A \vee \neg B \vee C) \wedge (\neg A \vee C \vee D) \wedge (B \vee D \vee \neg E) \wedge (\neg C \vee \neg D \vee \neg E) \wedge (\neg A \vee \neg C \vee E)$

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



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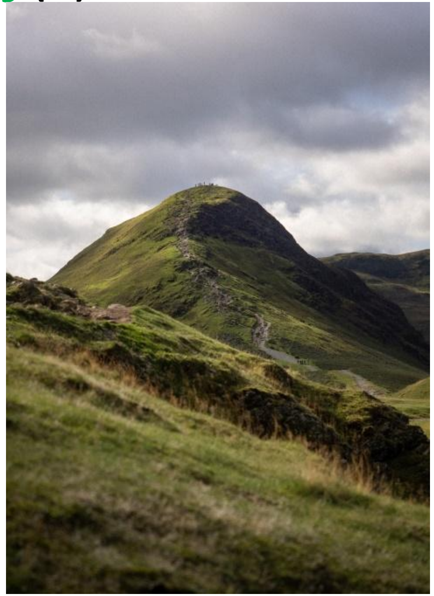
Hill Climbing

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.

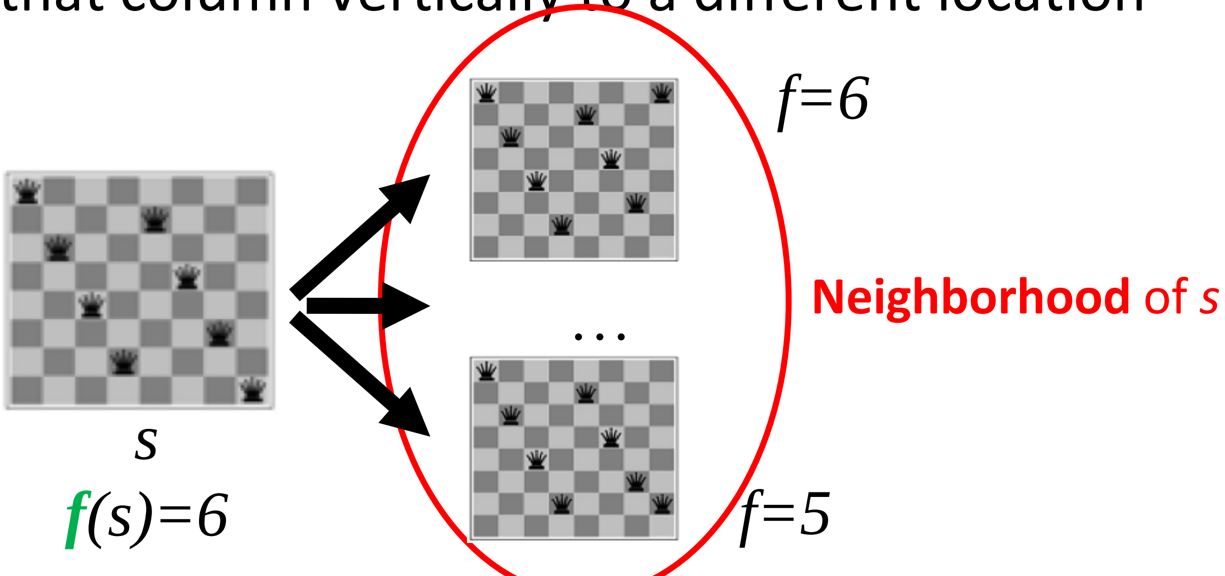
- **Q**: how do we define **neighbor**?
  - Not as obvious as our successors in search
  - Problem-specific
  - As we'll see, needs a careful choice



Defining Neighbors: n Queens

In n Queens, a simple possibility:

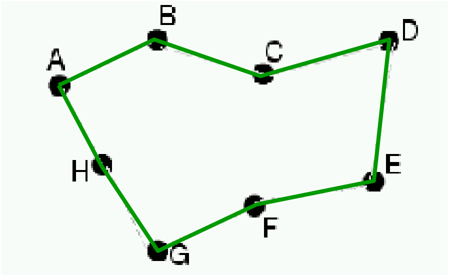
- Look at the **most-conflicting column** (ties? right-most one)
- Move queen in that column vertically to a different location



Defining Neighbors: TSP

For TSP, can do something similar:

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



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: (A=T, B=F, C=T, D=T, F=T)

(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**)

$A \vee \neg B \vee C$
$\neg A \vee C \vee D$
$B \vee D \vee \neg E$
$\neg C \vee \neg D \vee \neg E$
$\neg A \vee \neg C \vee E$

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**!
  - 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

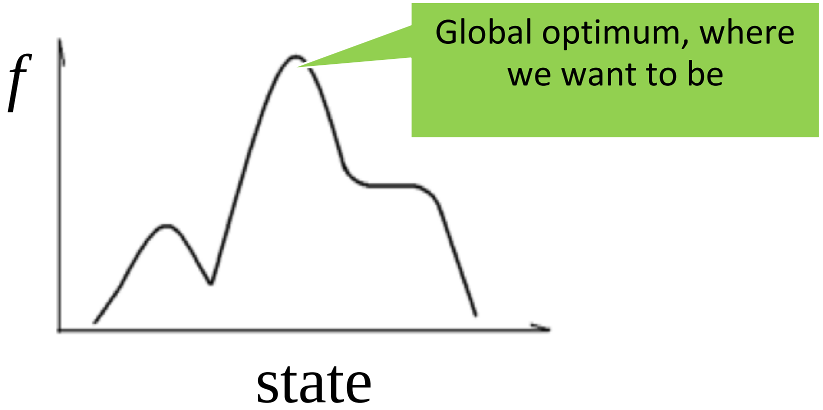
Pseudocode:

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* ← *t*. goto 2.

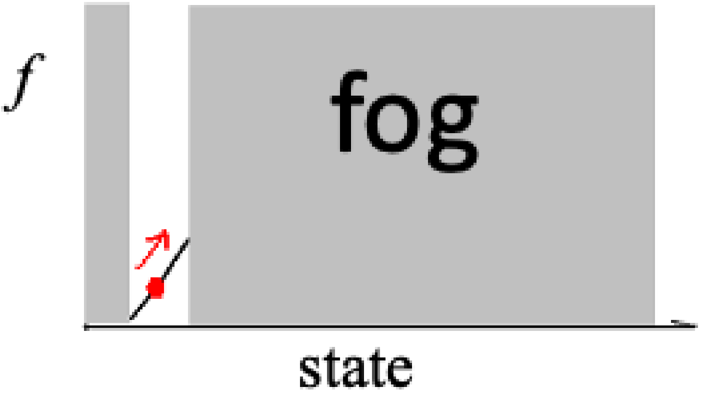
What could happen? **Local optima!**

Hill Climbing: Local Optima

Q: Why is it called hill climbing?



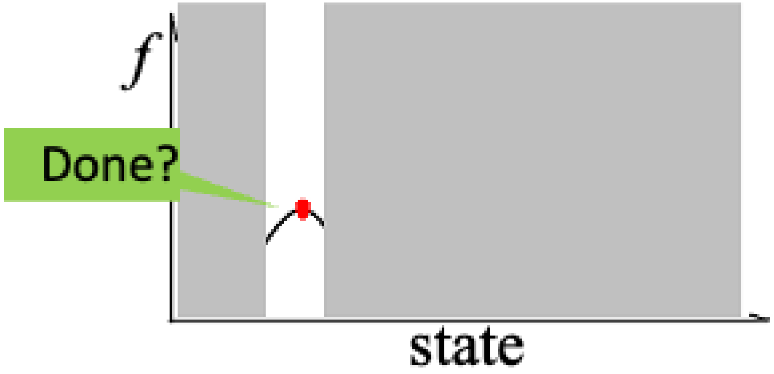
L: What's actually going on.

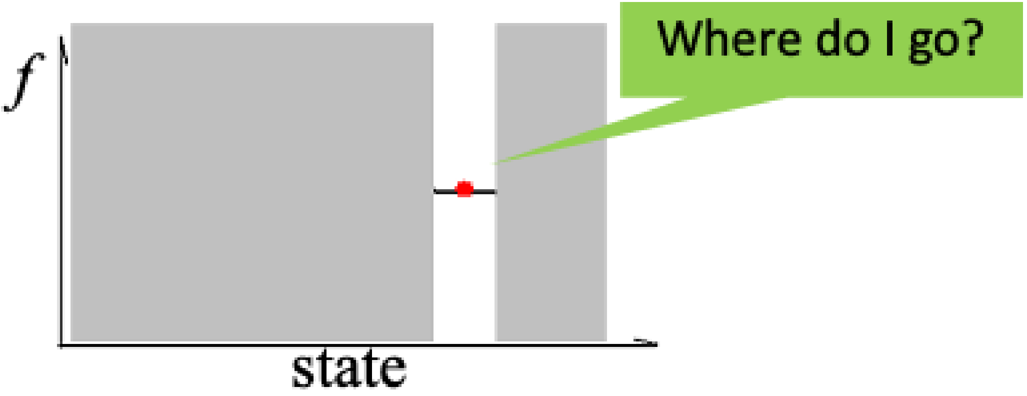


R: What we get to see.

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.

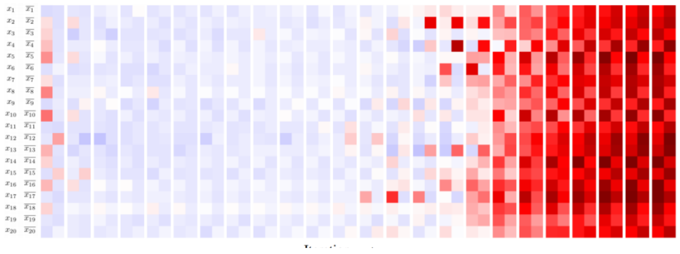
Hill Climbing: Variations

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



D. Selsam

Break & Quiz

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

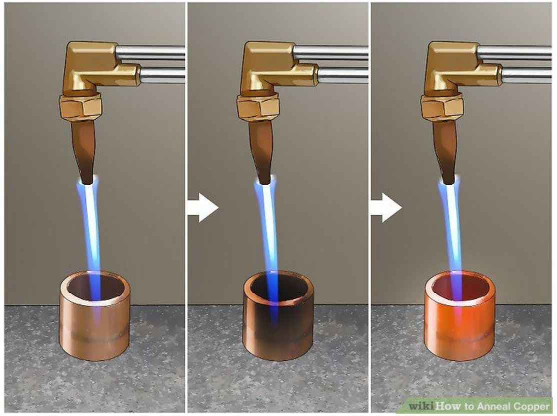
Simulated Annealing

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 ← T*0.99 (cool down)*
    Pick a random neighbour t ← neighbor(s)
    If $f(t)$ better than $f(s)$, then $s \leftarrow t$
    Else with prob. $P(f(s), f(t), \boldsymbol{T})$ still do $s \leftarrow t$
Output: the best state ever seen

The interesting bit



wikihow.com

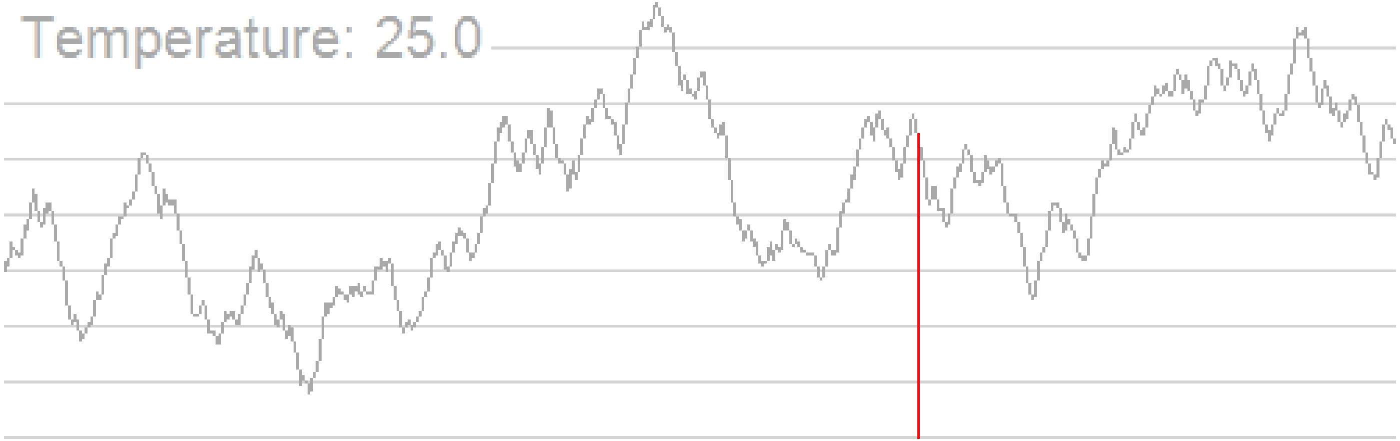
Simulated Annealing: Picking Probability

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?



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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

Break & Quiz

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. $Temp_{t+1} = Temp_t * 0.0001$

Break & Quiz

Q 2.2: Which of the following would be better to solve with hill climbing rather 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)

Genetic Algorithms

Optimization approach based on nature

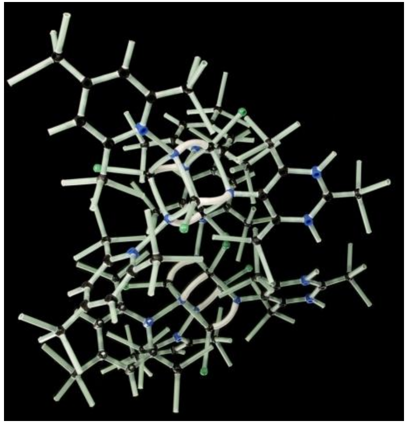
- Survival of the fittest!

Evolution Review

Encode genetic information in DNA (four bases)

- A/C/T/G: nucleobases acting as symbols

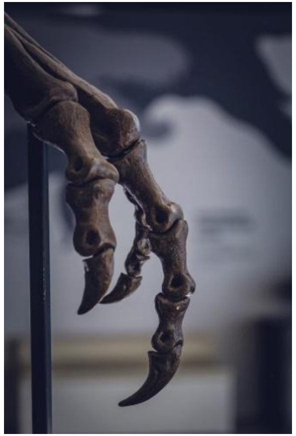
- Two types of changes
  - Crossover: exchange between parents' codes
  - Mutation: rarer random process
    - Happens at individual level



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

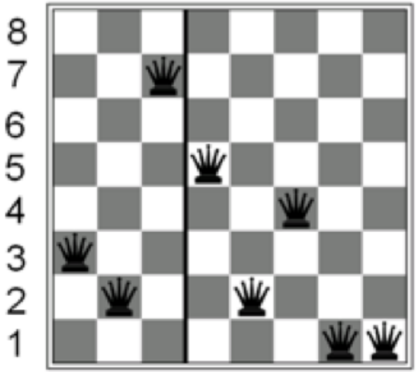
- New terminology: state is '**individual**'
- Value $f(s)$ is now the '**fitness**'

Genetic Algorithms Setup I

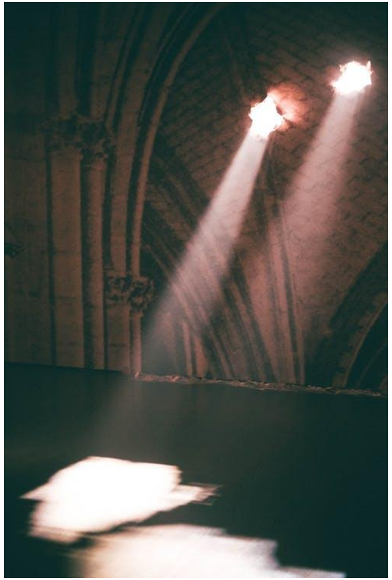
Keep around a fixed number of states/individuals

- Call this the **population**

For our n Queens game example, an individual:



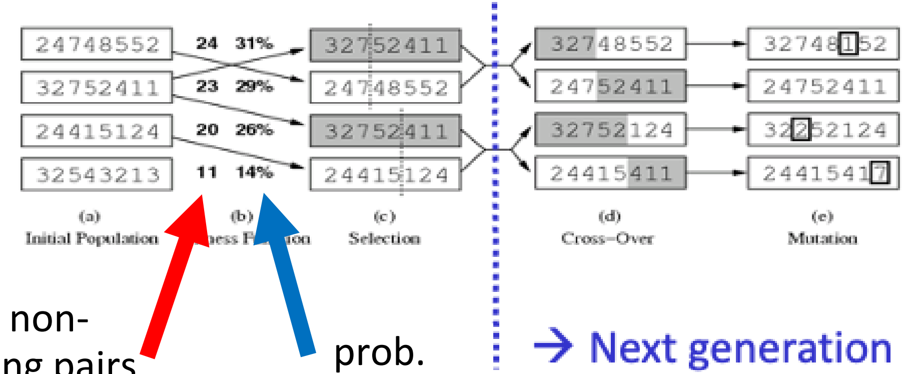
(3 2 7 5 2 4 1 1)



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 $s_1, \ldots, s_N$ 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%

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

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

$= \mathtt{MMFTM}$

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

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

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

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

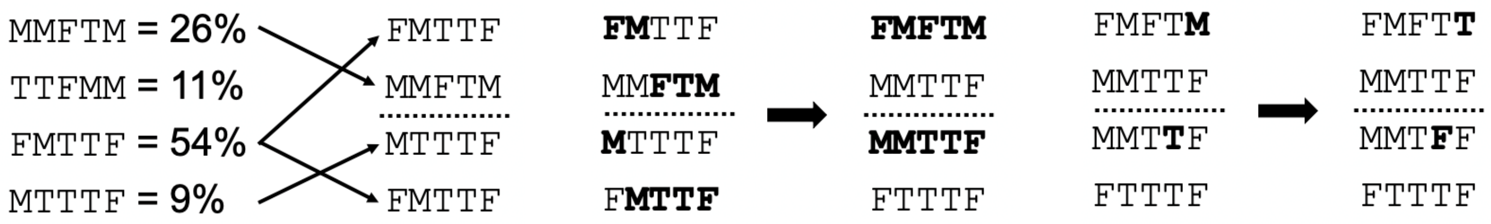
- Calculate reproduction probabilities

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
- 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