CS 540 Introduction to Artificial Intelligence
Search III: Advanced Search

University of Wisconsin-Madison

Spring 2022

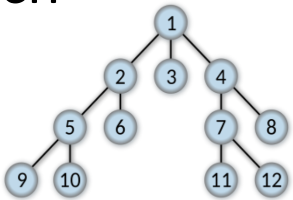
Outline

- 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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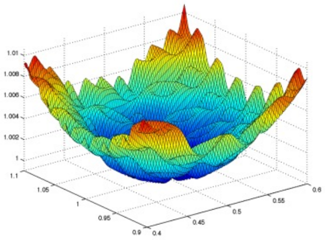

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New setting: optimization

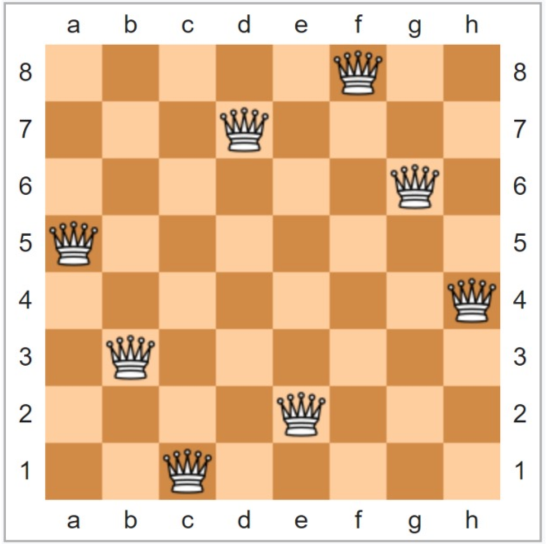
- States *s* have values ***f***(*s*)
- Want: *s* with optimal value ***f***(*s*) (i.e, **optimize** over states)
- Challenging setting: **too many states** for previous search approaches, but maybe not a differentiable function for SGD.

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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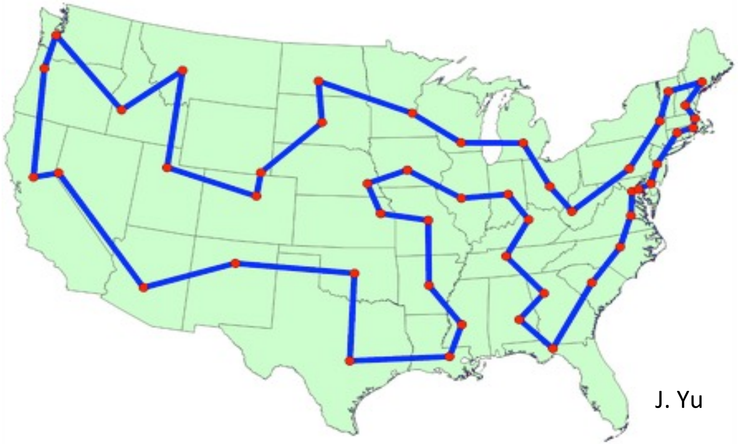
Examples: TSP

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)



J. Yu

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

$$\begin{array}{l}
R(x,a,d) \land R(y,b,d) \land R(a,b,e) \land R(c,d,f) \land R(z,c,0) \\
\hline
R(0,a,d) \land R(0,b,d) \land R(a,b,e) \land R(c,d,f) \land R(0,c,0) \\
R(0,a,d) \land R(0,b,d) \land R(a,b,e) \land R(c,d,f) \land R(1,c,0) \\
R(0,a,d) \land R(1,b,d) \land R(a,b,e) \land R(c,d,f) \land R(0,c,0) \\
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R(1,a,d) \land R(1,b,d) \land R(a,b,e) \land R(c,d,f) \land R(1,c,0)
\end{array}$$

$$\begin{array}{l}
R(\neg x,a,b) \land R(b,y,c) \land R(c,d,\neg z) \\
\hline
R(1,a,b) \land R(b,0,c) \land R(c,d,1) \\
R(1,a,b) \land R(b,0,c) \land R(c,d,0) \\
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\end{array}$$

Wiki

Hill Climbing

One approach to such optimization problems.

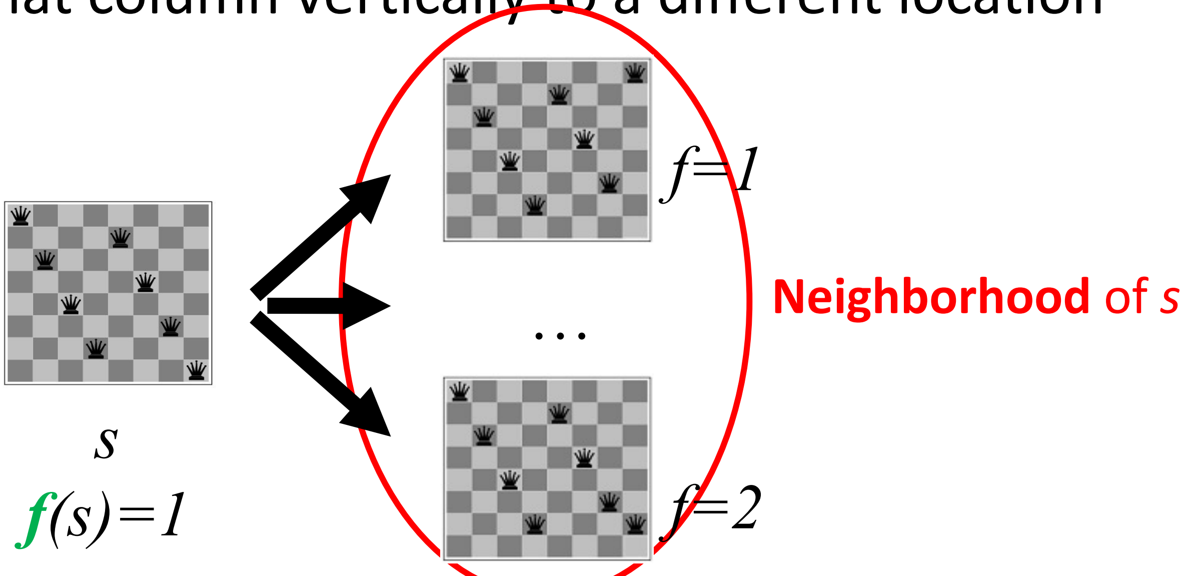
- Basic idea: move to a neighbor with a better ***f***(*s*)

- **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:

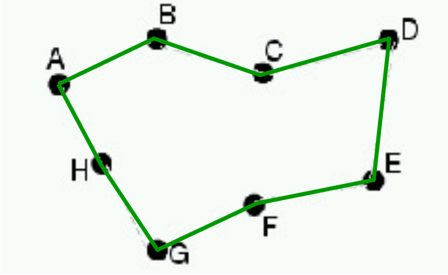
- Look at the **most-conflicting column** (ties? right-most one)
- Move queen in that column vertically to a different location



Defining Neighbors: TSP

For TSP, can do something similar:

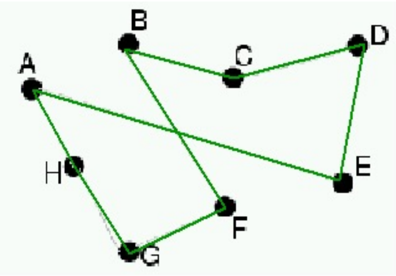
- Define neighbors by small changes
- Example: 2-change: A-E and B-F



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**)

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

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**!
  - 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

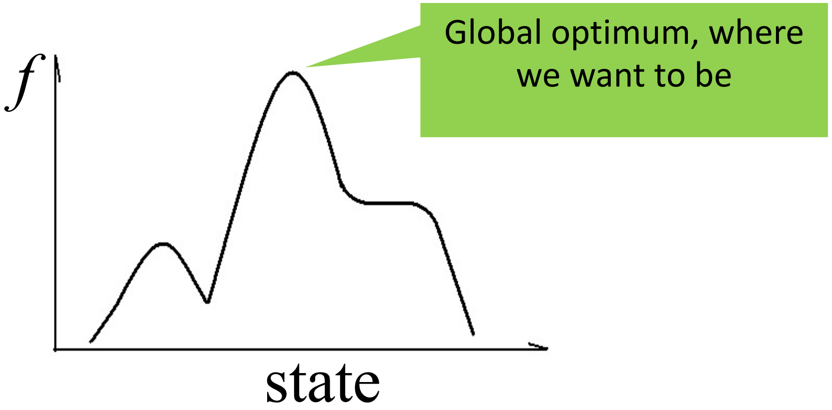
Pseudocode:

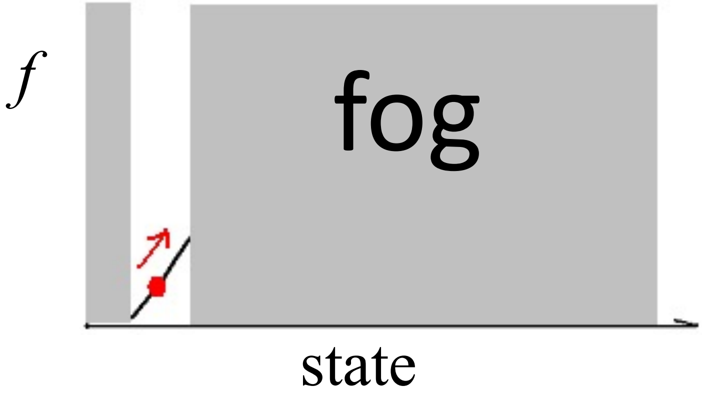
1. Pick initial state s
2. Pick t in **neighbors**(s) with the largest $\boldsymbol{f}(t)$
3. if $\boldsymbol{f}(t) \leq \boldsymbol{f}(s)$ THEN stop, return s
4. $s \leftarrow t$. goto 2.

What could happen? **Local optima!**

Hill Climbing: Local Optima

Q: Why is it called hill climbing?



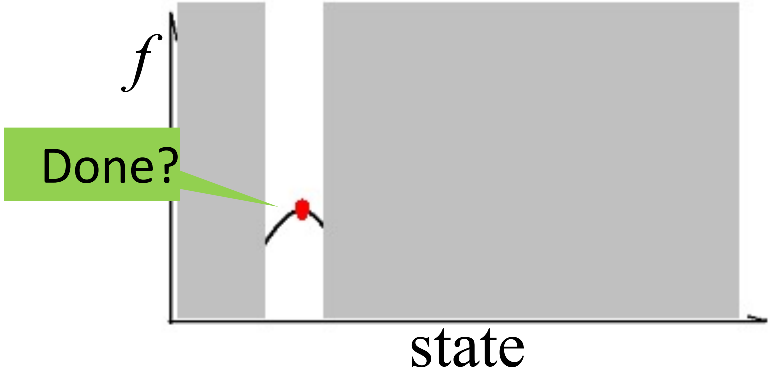


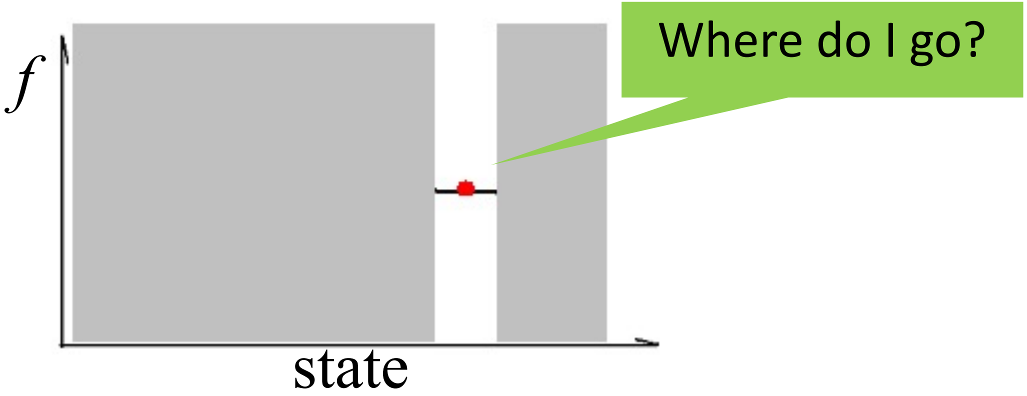
L: What's actually going on.

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

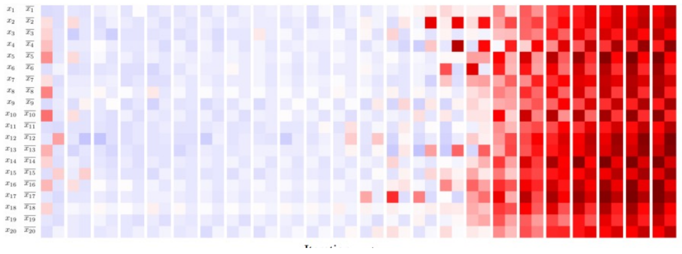
Hill Climbing: Variations

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



D. Selsam

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

Break & Quiz

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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.)

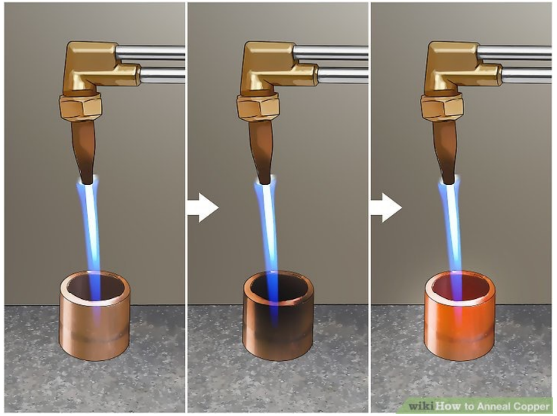
Simulated Annealing

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

The interesting bit



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Simulated Annealing: Picking Probability

How do we pick probability P(f(s), f(t), Temp)?

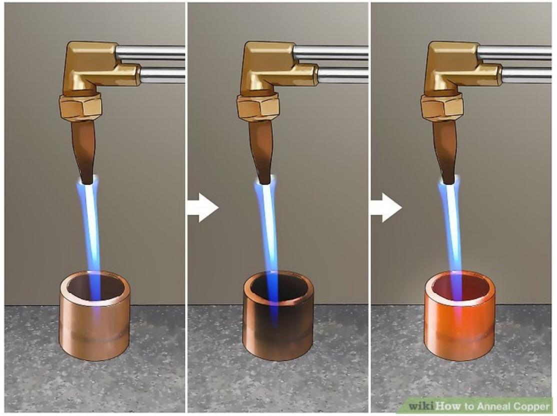
- Decrease with temperature
- Decrease with gap ***f***(*s*) - ***f***(*t*):

$$\exp\left(-\frac{|f(s)-f(t)|}{Temp}\right)$$

- 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: 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



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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 2.1: 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 2.1: 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)

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

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

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

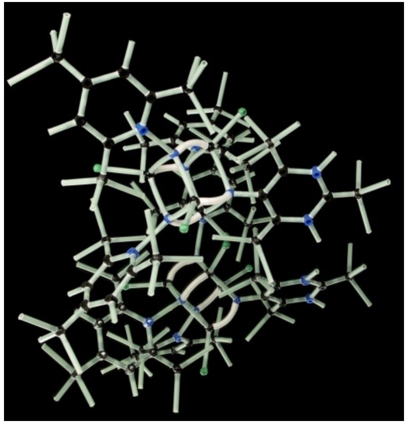
- Survival of the fittest!

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

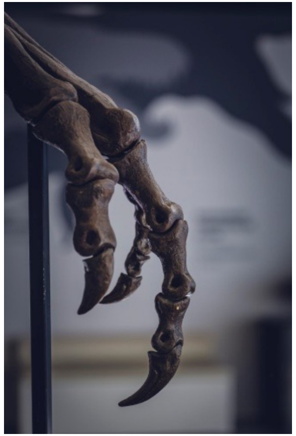
Competition for resources

- Organisms better fit ➔ 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**’

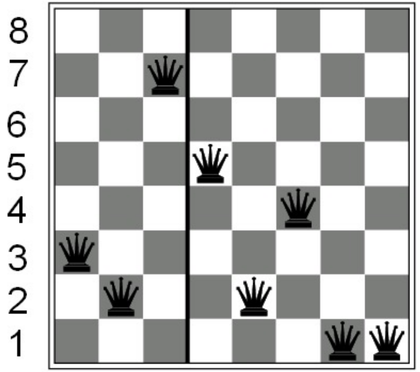


Genetic Algorithms Setup I

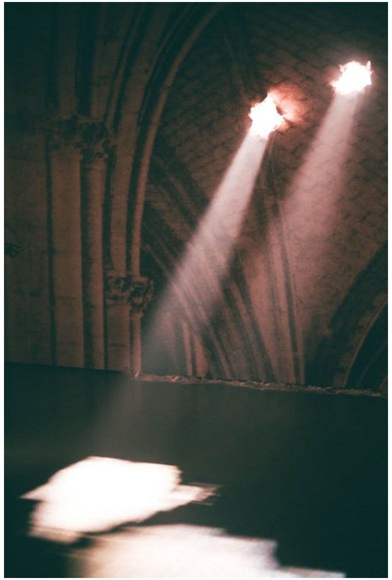
Keep around a fixed number of states/individuals

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

For our n Queens game example, an individual:



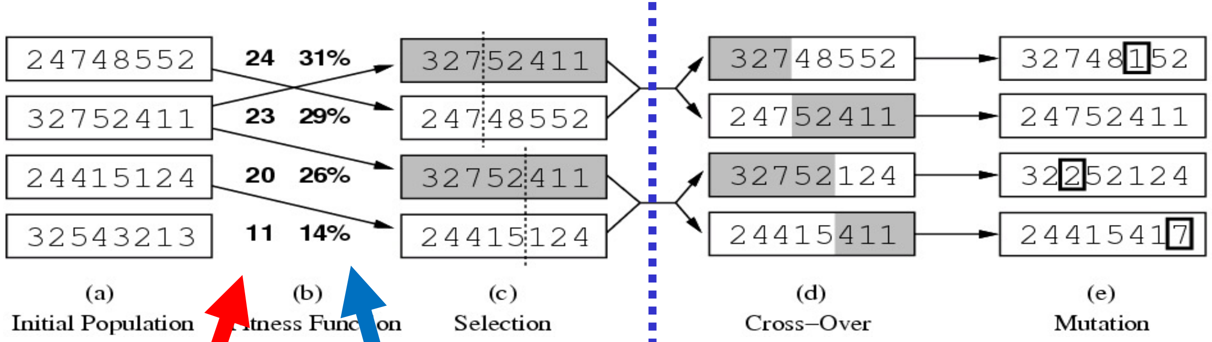
(3 2 7 5 2 4 1 1)



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**



# 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 $p_i = f(s_i) \,/\, \Sigma_j\, f(s_j)$ 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: $p_i = \boldsymbol{f}(s_i) \,/\, \Sigma_j\, \boldsymbol{f}(s_j)$

- **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%

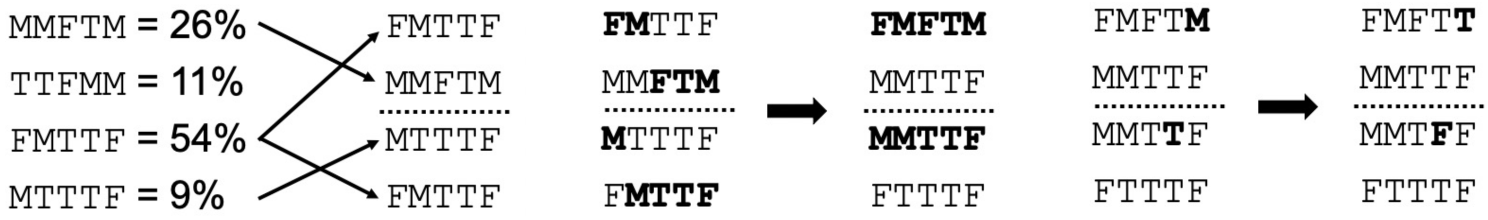
- Calculate reproduction probabilities

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**

- 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