# Advanced Search

## Hill climbing, simulated annealing, genetic algorithm

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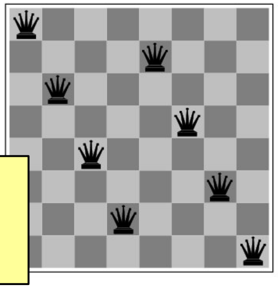
Based on slides from Andrew Moore
(https://www.autonlab.org/resources/tutorials), modified
by Xiaojin Zhu (UW-Madison) and Anthony Gitter

# Optimization problems

- Previously we want a path from start to goal
  - Uninformed search: g(s): Iterative Deepening
  - Informed search: g(s)+h(s): A*
- **Now a different setting**:
  - Each state *s* has a score *f(s)* that we can compute
  - The goal is to find the state with the highest score, or a reasonably high score
  - Do not care about the path
  - This is an optimization problem
  - Enumerating the states is intractable
  - Even previous search algorithms are too expensive

# Examples

- N-queen: *f*(*s*) = number of conflicting queens in state *s*



Note we want *s* with the lowest score *f*(*s*)=0. The techniques are the same. Low or high should be obvious from context.

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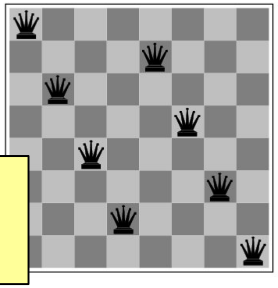
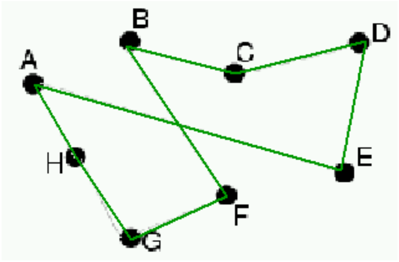


- Traveling salesperson problem (TSP)
  - Visit each city once, return to first city
  - State = order of cities, *f*(*s*) = total mileage



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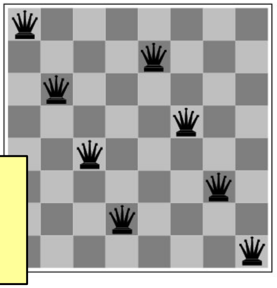

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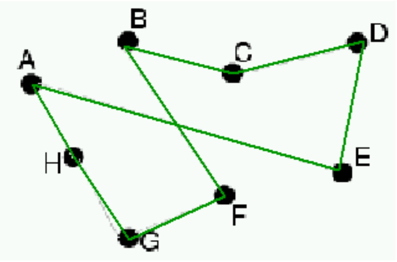


- Boolean satisfiability (e.g., 3-SAT)
  - State = assignment to variables
  - $f(s)$ = # satisfied clauses
  - $\vee$ means OR

$A \vee \neg B \vee C$
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**Note: the recorded lecture incorrectly discussed clauses with AND operators instead of OR**

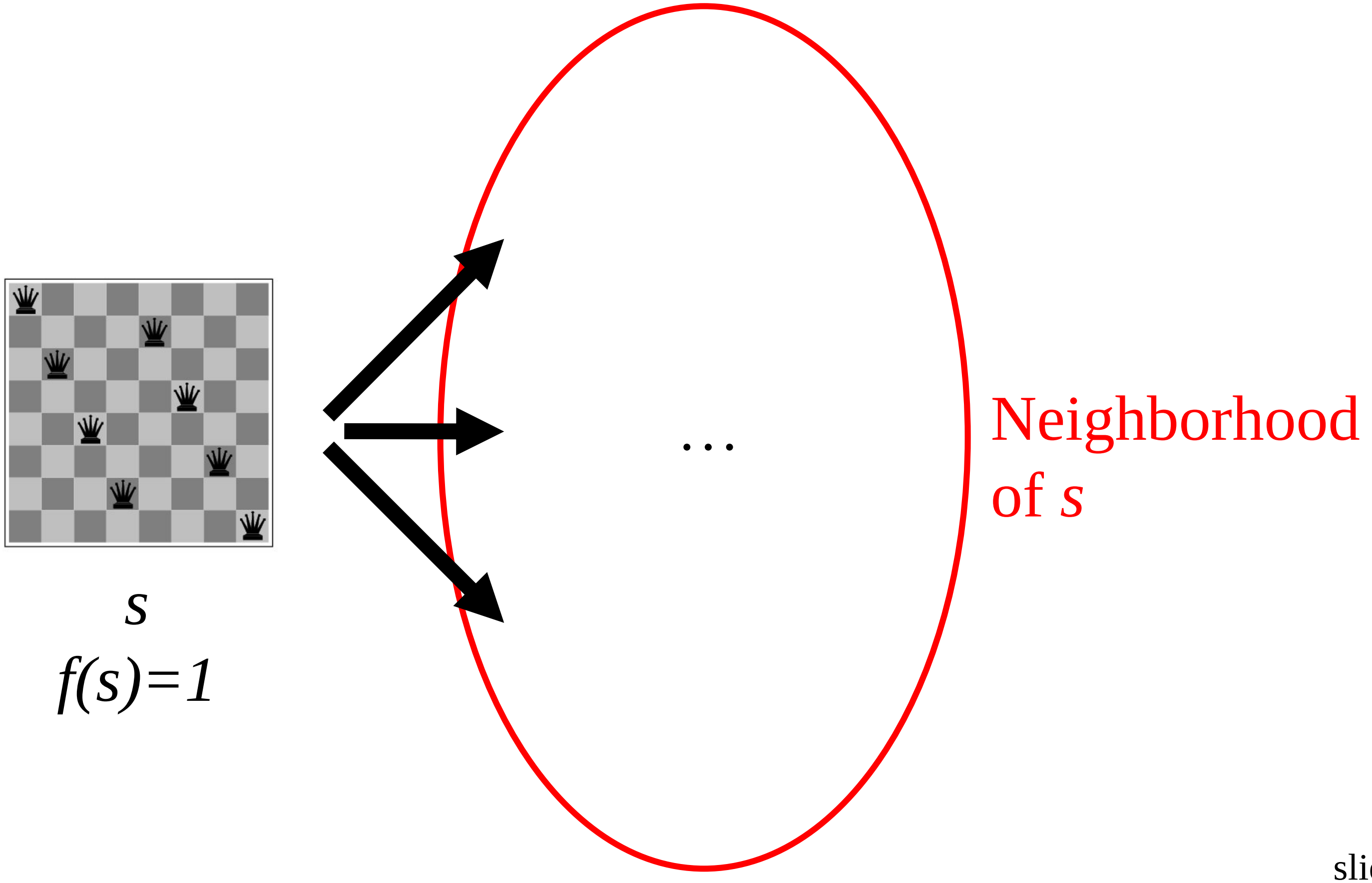
# 1. HILL CLIMBING

# Hill climbing

- Very simple idea: Start from some state *s*,
  - Move to a neighbor *t* with better score. Repeat.
- **Question**: what's a neighbor?
  - You have to define that!
  - The neighborhood of a state is the set of neighbors
  - Also called 'move set'
  - Similar to successor function

# Neighbors: N-queen

- Example: N-queen (one queen per column). One possibility:




*s*
*f(s)=1*

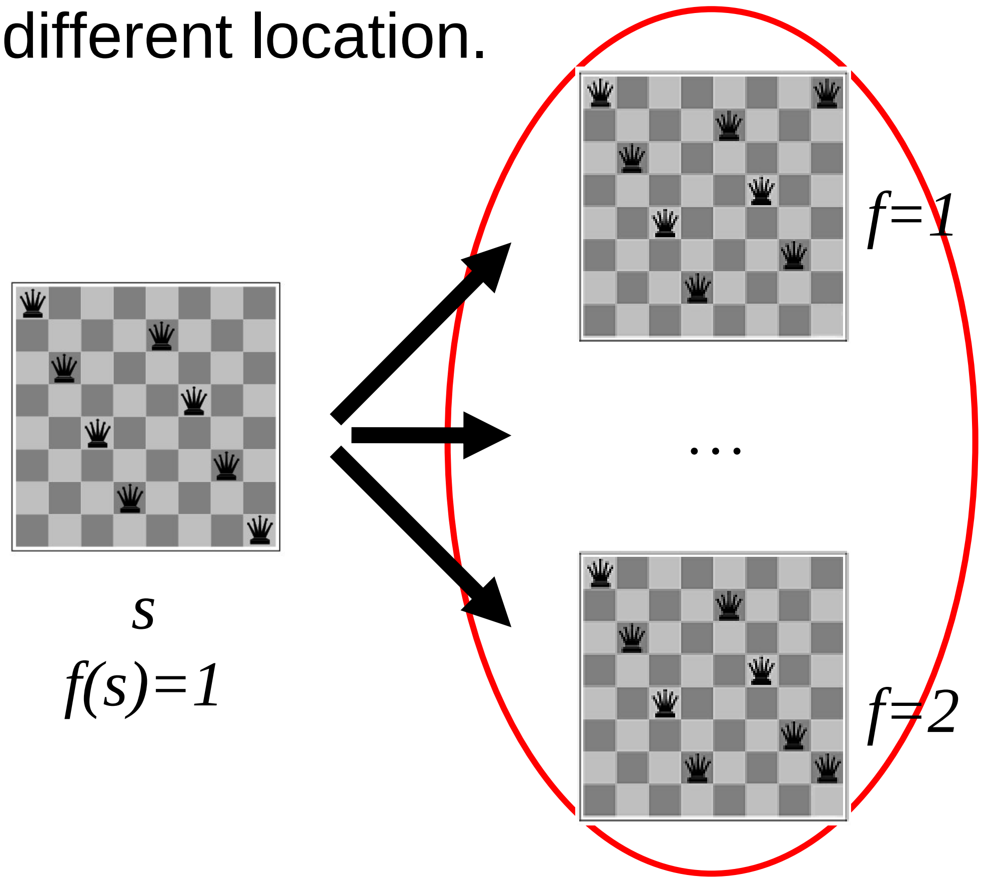
# Neighbors: N-queen

- Example: N-queen (one queen per column). One possibility:

  tie breaking

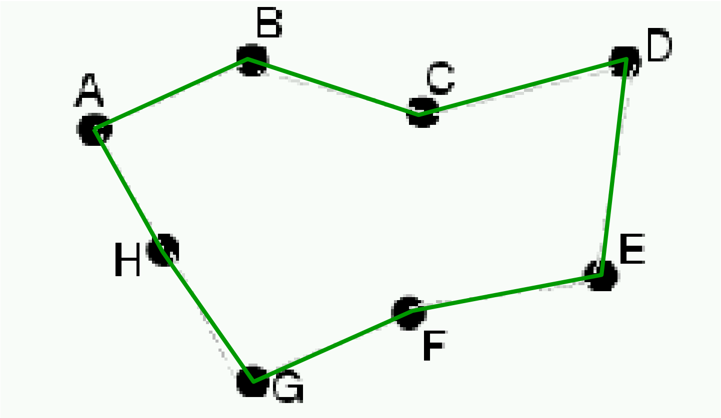
  more promising?

  - Pick the right-most most-conflicting column;
  - Move the queen in that column vertically to a different location.



# Neighbors: TSP

- state: A-B-C-D-E-F-G-H-A
- *f* = length of tour



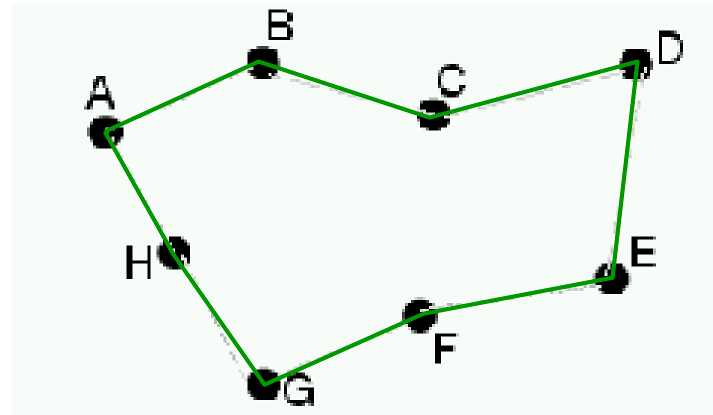
# Neighbors: TSP

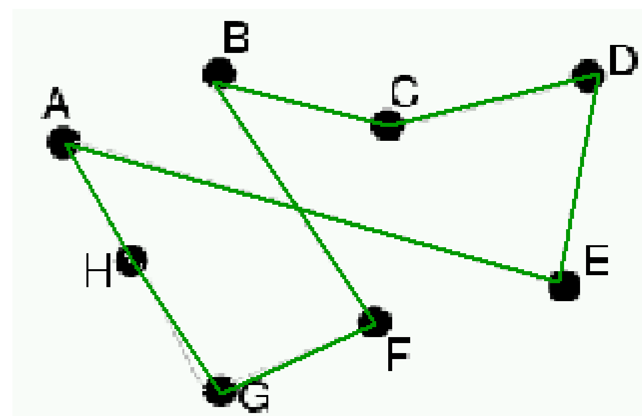
- state: A-B-C-D-E-F-G-H-A
- *f* = length of tour
- One possibility: 2-change

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

flip

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



# Neighbors: SAT

- State: (A=T, B=F, C=T, D=T, E=T)
- *f* = number of satisfied clauses
- Neighbor:

$A \lor \neg B \lor C$
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- State: (A=T, B=F, C=T, D=T, E=T)
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- Neighbor: flip the assignment of one variable

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(A=T, B=**T**, C=T, D=T, E=T)
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(A=T, B=F, C=T, D=**F**, E=T)
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# Hill climbing

- **Question**: What's a neighbor?
  - (vaguely) Problems tend to have structures. A small change produces a neighboring state.
  - The neighborhood must be small enough for efficiency
  - Designing the neighborhood is critical. This is the real ingenuity – not the decision to use hill climbing.
- **Question**: Pick which neighbor?
- **Question**: What if no neighbor is better than the current state?

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  - The neighborhood must be small enough for efficiency
  - Designing the neighborhood is critical. This is the real ingenuity – not the decision to use hill climbing.
- **Question**: Pick which neighbor? The best one (greedy)
- **Question**: What if no neighbor is better than the current state? Stop.

# Hill climbing algorithm

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* = *t*. GOTO 2.

- Not the most sophisticated algorithm in the world.
- Very greedy.
- Easily stuck.

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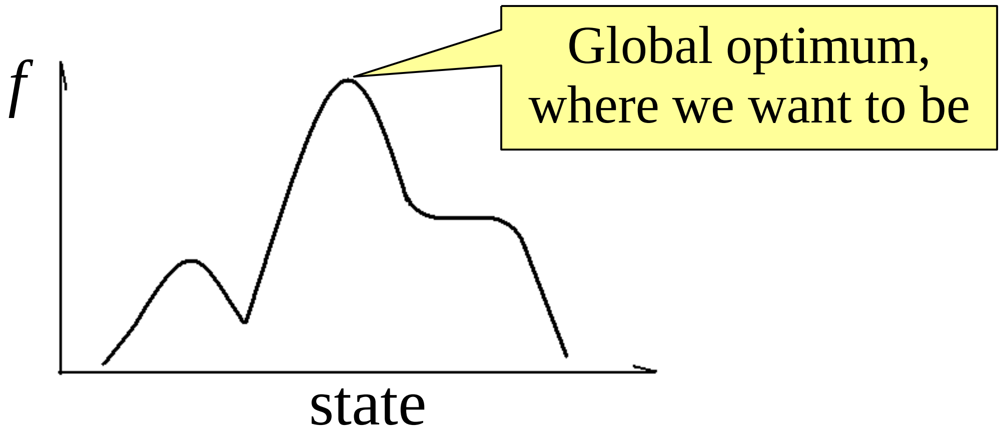
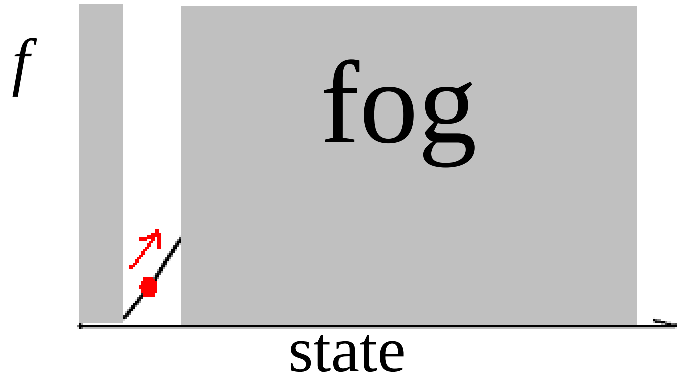
your enemy:
local
optima

# Local optima in hill climbing

- Useful conceptual picture: *f* surface = ‘hills’ in state space

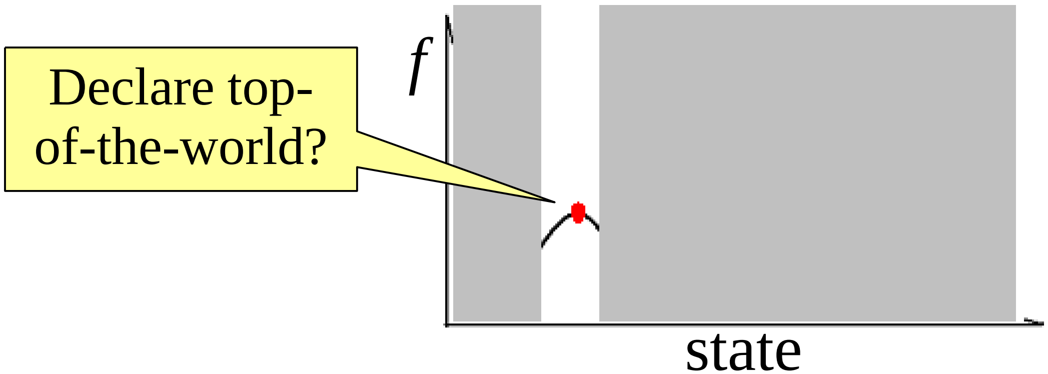



- But we can’t see the landscape all at once.  Only see the neighborhood.  Climb in fog.

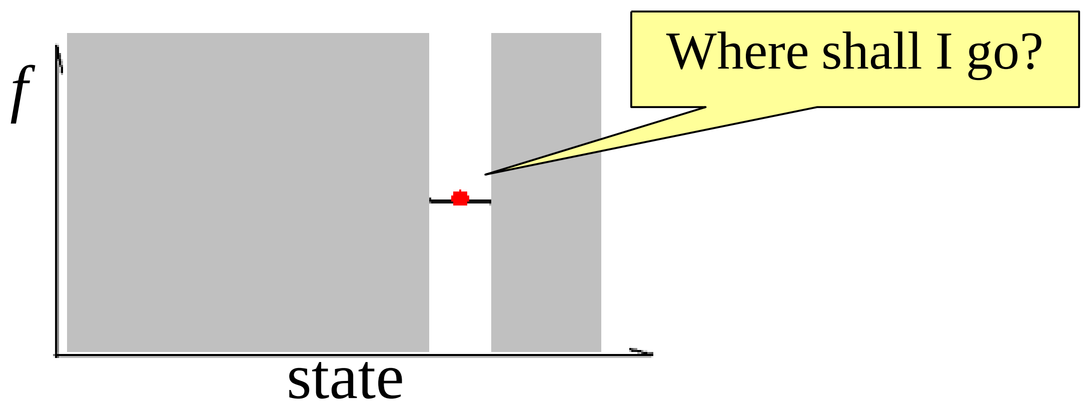


# Local optima in hill climbing

- Local optima (there can be many!)




- Plateaux



# Local optima in hill cl mbing

- Local optima (there ca e ma

Declare
of-the-wo

$f$

- Plate

ere shall I go?

e

We'll learn
strategies for
**escaping**
**local optima**

# Not every local minimum should be escaped

# Example: Hill climbing for SAT

- $f$ = number of satisfied clauses
- Neighbor: flip the assignment of one variable

| State | $f$ |
|---|---|
| (A=T, B=T, C=T, D=T, E=T) | 0 |

$A \vee \neg B \vee C$
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| (A=T, B=T, C=T, D=T, E=**F**) | 1 |

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Stuck

Is this the global optimum?

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What if we had picked a different neighbor?

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Stuck

Is this the global optimum?

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# Repeated hill climbing with random restarts

- Very simple modification

  1. When stuck, pick a random new start, run basic hill climbing from there.
  2. Repeat this *k* times.
  3. Return the best of the *k* local optima.

- Can be very effective
- Should be tried whenever hill climbing is used

# Variations of hill climbing

- **Question**: How do we make hill climbing less greedy?

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  - Stochastic hill climbing
    - Randomly select among better neighbors
    - The better, the more likely
    - Pros / cons compared with basic hill climbing?

# Variations of hill climbing

- **Question**: What if the neighborhood is too large to enumerate? (e.g. N-queen if we need to pick both the column and the move within it)

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- **Question**: What if the neighborhood is too large to enumerate? (e.g. N-queen if we need to pick both the column and the move within it)
  - First-choice hill climbing
    - Randomly generate neighbors, one at a time
    - If better, take the move
    - Pros / cons compared with basic hill climbing?

# Variations of hill climbing

- We are still greedy!  Only willing to move upwards.
- Important observation in life:

| | | |
|---|---|---|
| Sometimes one needs to temporarily step back in order to move forward. | = | Sometimes one needs to move to an inferior neighbor in order to escape a local optimum. |

# Variations of hill climbing

WALKSAT [Selman]

- Pick a random unsatisfied clause
- Consider 3 neighbors: flip each variable
- If any improves *f*, accept the best
- If none improves *f*:
  - 50% of the time pick the least bad neighbor
  - 50% of the time pick a random neighbor

This is the best known algorithm for satisfying Boolean formulae.

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# 2. SIMULATED ANNEALING

# Simulated Annealing

**anneal**

- To subject (glass or metal) to a process of heating and slow cooling in order to toughen and reduce brittleness.

# Simulated Annealing

1. Pick initial state *s*
2. Randomly pick *t* in neighbors(*s*)
3. IF *f*(*t*) better THEN accept *s*🡐*t*.
4. ELSE /* *t* is worse than *s* */
5. accept *s*🡐*t* with a small probability
6. GOTO 2 until bored.

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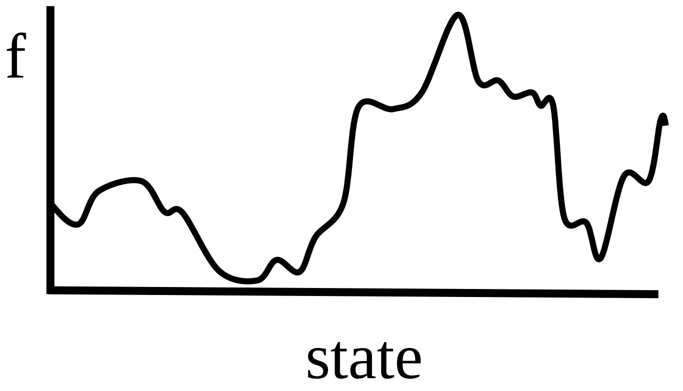
How to choose the small probability?

idea 1: $p = 0.1$



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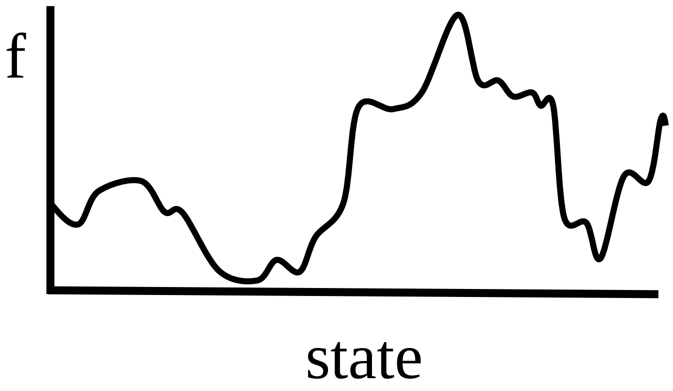

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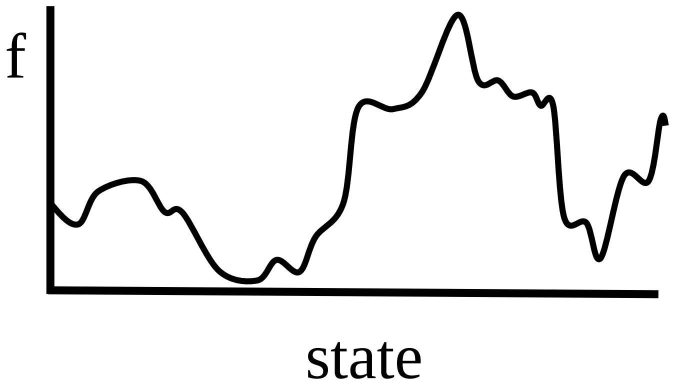
idea 3: $p$ decreases with time, also as the 'badness' $|f(s)-f(t)|$ increases



# Simulated Annealing

- If *f*(*t*) better than *f*(*s*), always accept *t*
- Otherwise, accept *t* with probability

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

Boltzmann distribution

# Simulated Annealing

- If $f(t)$ better than $f(s)$, always accept $t$
- Otherwise, accept $t$ with probability

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

Boltzmann distribution

- *Temp* is a temperature parameter that 'cools' (anneals) over time, e.g. $Temp \leftarrow Temp*0.9$ which gives $Temp=(T_0)^{\#iteration}$
  - High temperature: almost always accept any $t$
  - Low temperature: first-choice hill climbing
- If the 'badness' (formally known as energy difference) $|f(s)-f(t)|$ is large, the probability is small.

# Simulated Annealing algorithm

// assuming we want to maximize f()

current = Initial-State(problem)

**for** t = 1 **to** ∞ **do**

T = Schedule(t) ; // T is the current temperature, which is monotonically decreasing with t

**if** T=0 **then return** current ; // halt when temperature = 0

next = Select-Random-Successor-State(current)

deltaE = f(next) - f(current) ; // If positive, next is better than current. Otherwise, next is worse than current.

**if** deltaE > 0 **then** current = next ; // always move to a better state

**else** current = next with probability p = exp(deltaE / T) ;
// as T → 0, p → 0; as deltaE → -∞, p →0

**end**

# Simulated Annealing issues

- Cooling scheme important
- Neighborhood design is the real ingenuity, not the decision to use simulated annealing.
- Not much to say theoretically
  - With infinitely slow cooling rate, finds global optimum with probability 1.
- Proposed by **Metropolis** in 1953 based on the analogy that alloys manage to find a near global minimum energy state, when annealed slowly.
- Easy to implement.
- Try hill-climbing with random restarts first!

# 3. GENETIC ALGORITHM


Image: Elliott Kalan, Marco Failla/Marvel Comics

# Evolution

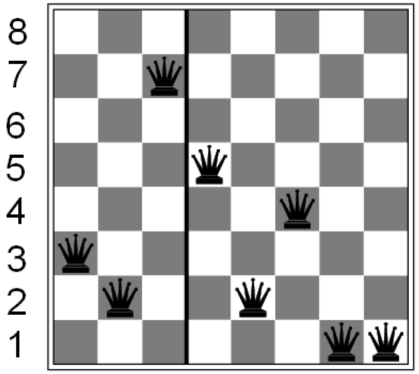
- Survival of the fittest, a.k.a. natural selection
- Genes encoded as DNA (deoxyribonucleic acid), sequence of bases: A (Adenine), C (Cytosine), T (Thymine) and G (Guanine)
- The chromosomes from the parents exchange randomly by a process called **crossover**. Therefore, the offspring exhibit some traits of the father and some traits of the mother.
  - Requires genetic diversity among the parents to ensure sufficiently varied offspring
- A rarer process called **mutation** also changes the genes (e.g. spontaneous from radiation).
  - Organisms with nonsensical/deadly mutated die.
  - Beneficial mutations produce “stronger” organisms.
  - Neither: organisms aren’t improved.

# Natural selection

- Individuals compete for resources
- Individuals with better genes have a larger chance to produce offspring, and vice versa
- After many generations, the population consists of more genes from the superior individuals, and less from the inferior individuals
- Superiority defined by fitness to the environment
- Popularized by Darwin, independently Wallace

# Genetic algorithm

- Yet another AI algorithm based on real-world analogy
- Yet another heuristic stochastic search algorithm
- Each state *s* is called an individual. Often (carefully) coded up as a string.




(3 2 7 5 2 4 1 1)

- The score *f*(*s*) is called the fitness of *s*. Our goal is to find the global optimum (fittest) state.
- At any time we keep a fixed number of states. They are called the population. Similar to beam search.

# Individual encoding

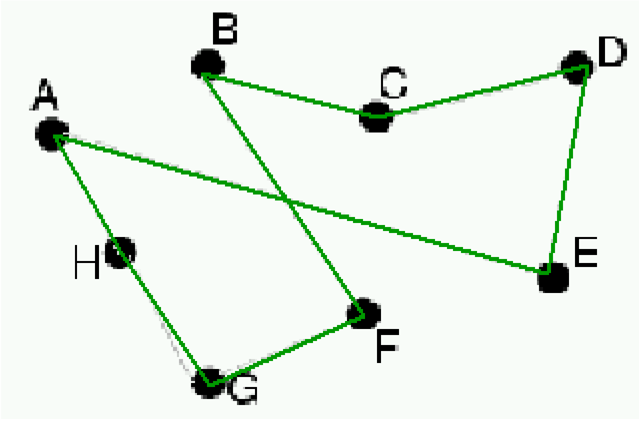
- The "DNA"
- Satisfiability problem

  (A B C D E) = (T F T T T)

- TSP

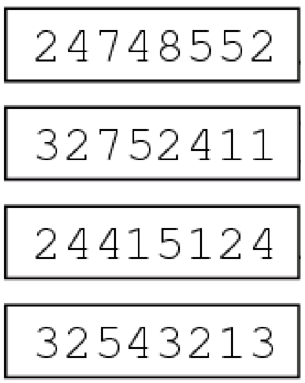
  A-E-D-C-B-F-G-H-A

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



# Genetic algorithm

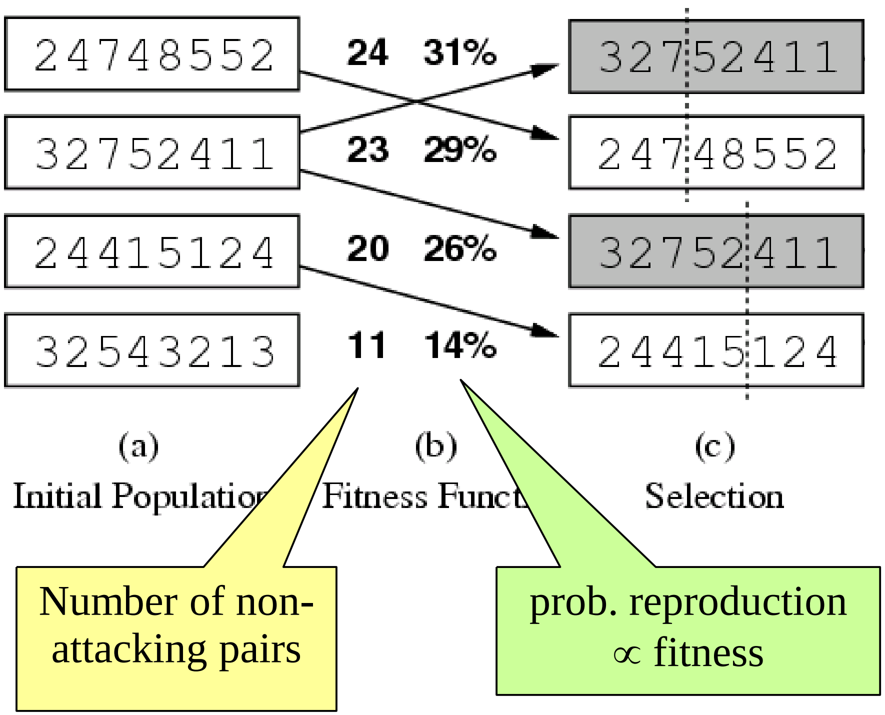
- **Genetic algorithm**: a special way to generate neighbors, using the analogy of cross-over, mutation, and natural selection.




(a)
Initial Population

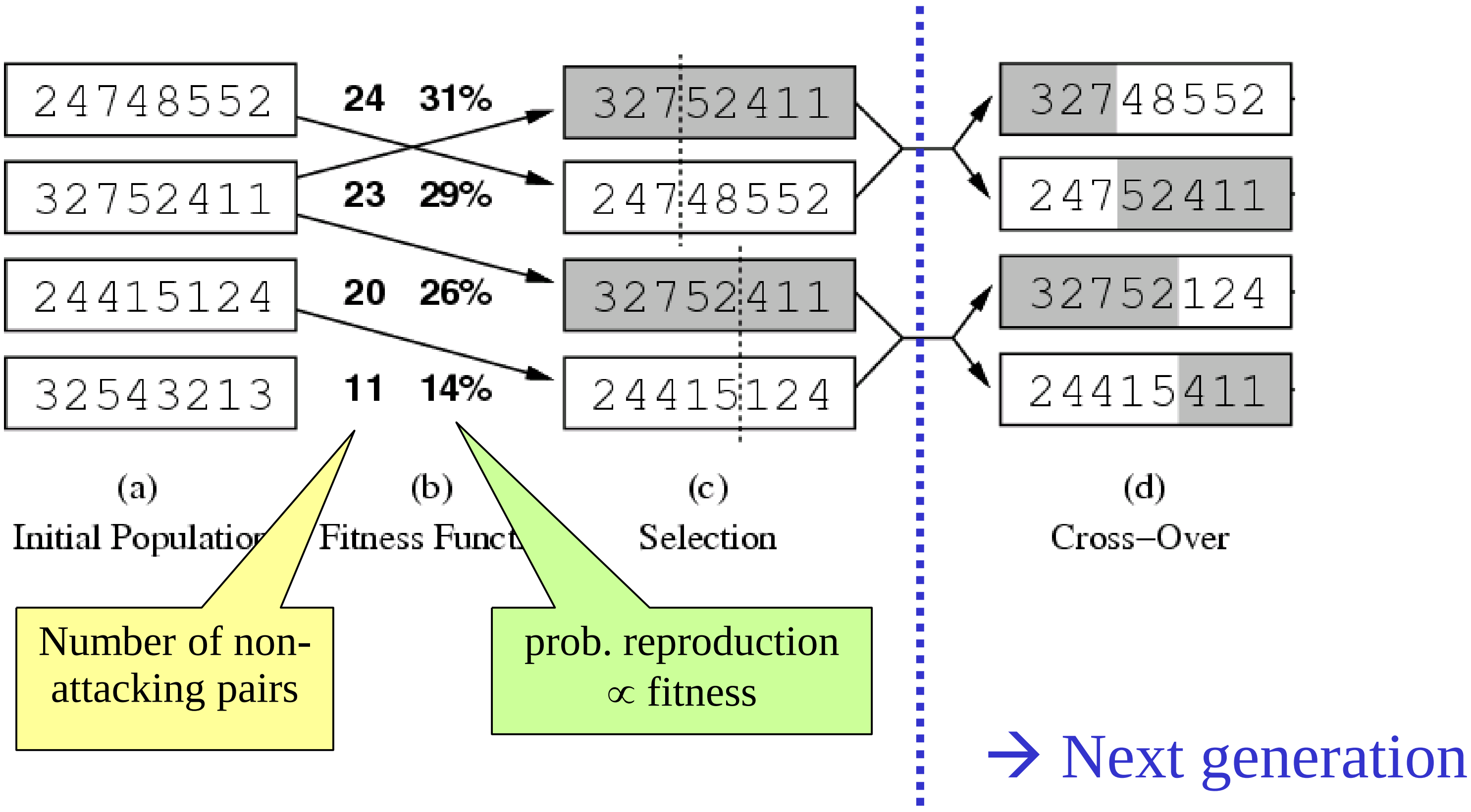
# Genetic algorithm

- **Genetic algorithm**: a special way to generate neighbors, using the analogy of cross-over, mutation, and natural selection.



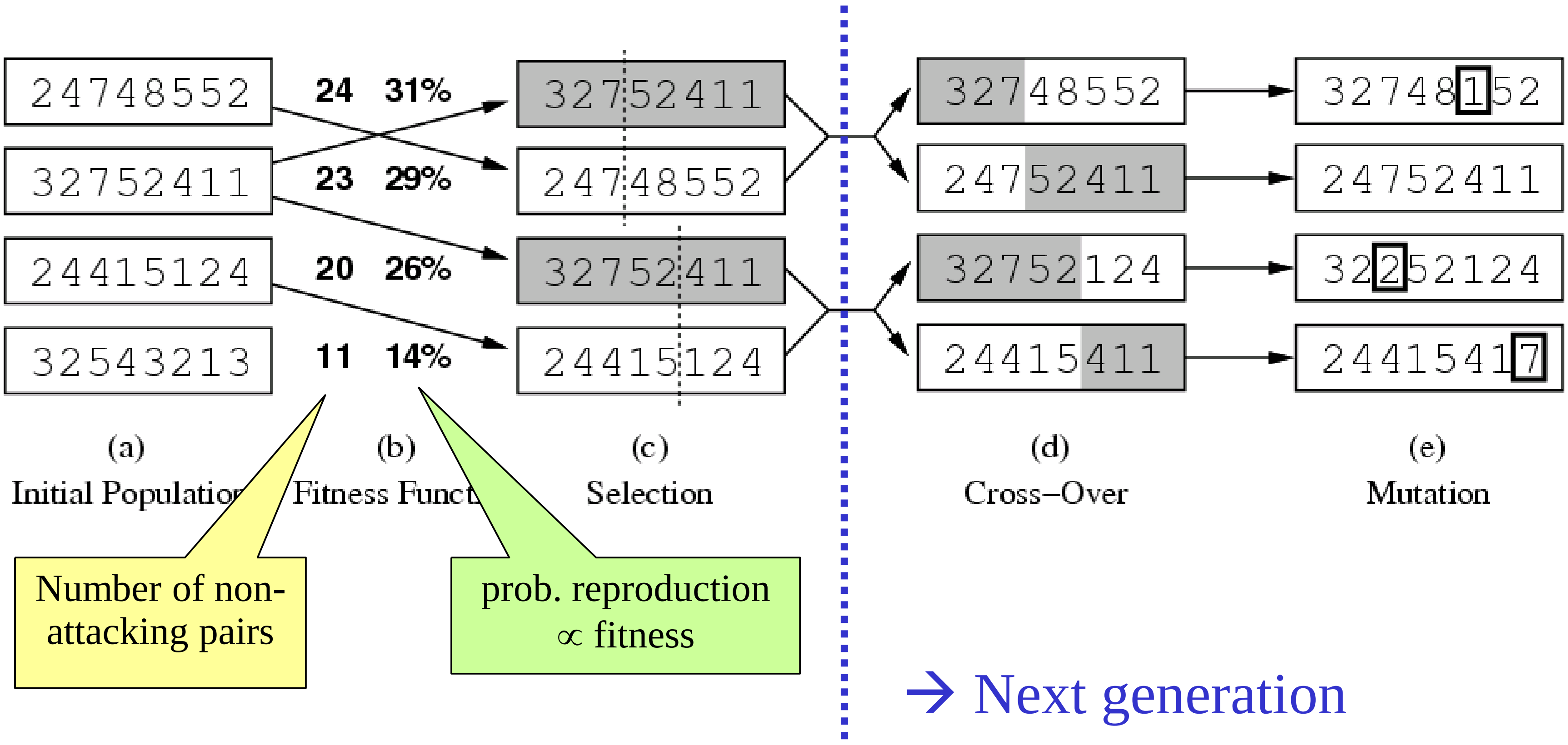
# Genetic algorithm

- **Genetic algorithm**: a special way to generate neighbors, using the analogy of cross-over, mutation, and natural selection.



# Genetic algorithm

- **Genetic algorithm**: a special way to generate neighbors, using the analogy of cross-over, mutation, and natural selection.



# Genetic algorithm (one variety)

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 = 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 until bored or state with good enough score.

# Proportional selection

- $p_i = f(s_i) / \Sigma_j f(s_j)$
- $\Sigma_j f(s_j) = 5+20+11+8+6=50$
- $p_1$=5/50=10%

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

# Genetic algorithm example

- Scheduling summer courses
- 5 courses: A, B, C, D, E
- 3 time slots (all day long): <u>M</u>on/Wed, <u>T</u>ue/Thu, <u>F</u>ri/Sat
- Students want to enroll in 3 courses

| 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 |

- Maximize students who can enroll in desired courses

# Genetic algorithm example

- State: assign each course to a time slot
- Courses: A, B, C, D, E
- Time slots: M, T, F

| M | M | F | T | M |
|---|---|---|---|---|
| A | B | C | D | E |

= MMFTM

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

# Genetic algorithm example

- Scoring a state `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 |

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

# Genetic algorithm example

- Randomly initialize and score states

  `MMFTM` = 9

  `TTFMM` = 4

  `FMTTF` = 19

  `MTTTF` = 3

- Calculate reproduction probabilities

  `MMFTM` = 26%

  `TTFMM` = 11%

  `FMTTF` = 54%

  `MTTTF` = 9%

| 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 |

# Genetic algorithm example

- Select parents using reproduction probabilities

| | |
|---|---|
| MMFTM = 26% | FMTTF |
| TTFMM = 11% | MMFTM |
| FMTTF = 54% | MTTTF |
| MTTTF = 9% | FMTTF |

- Cross-over to generate children

| | |
|---|---|
| **FM**TTF | **FMFTM** |
| MM**FTM** | MMTTF |
| **M**TTTF | **MMTTF** |
| F**MTTF** | FTTTF |

# Genetic algorithm example

- Randomly mutate new children

| | | |
|---|---|---|
| FMFT**M** | | FMFT**T** |
| MMTTF | | MMTTF |
| ............... | → | ............... |
| MMT**T**F | | MMT**F**F |
| FTTTF | | FTTTF |

# Genetic algorithm example

- Score states in updated population

  `FMFTT` = 11

  `MMTTF` = 13

  `MMTFF` = 4

  `FTTTF` = 0

- Calculate reproduction probabilities

  `FMFTT` = 39%

  `MMTTF` = 46%

  `MMTFF` = 14%

  `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 |

# Genetic algorithm example

- Select parents using reproduction probabilities

| | |
|---|---|
| FMFTT = 39% | FMFTT |
| MMTTF = 46% | MMTFF |
| MMTFF = 14% | FMFTT |
| FTTTF = 0% | MMTTF |

- Cross-over to generate children

| | |
|---|---|
| **FMFT**T | **FMFTF** |
| MMTF**F** | MMTFT |
| **F**MFTT | **FMTTF** |
| M**MTTF** | MMFTT |

# Genetic algorithm example

- Randomly mutate new children

| | | |
|---|---|---|
| FMFTF | | FMFTF |
| **M**MT**F**T | → | **F**MT**M**T |
| FMT**T**F | | FMT**M**F |
| MMFT**T** | | MMFT**F** |

- Continue iterating

# Variations of genetic algorithm

- Parents may survive into the next generation
- Use ranking instead of $f(s)$ in computing the reproduction probabilities
- Cross over random bits instead of chunks
- Optimize over sentences from a programming language.  Genetic programming.
- …

# Genetic algorithm issues

- State encoding is the real ingenuity, not the decision to use genetic algorithm
- Lack of diversity can lead to premature convergence and non-optimal solution
- Have to pick several parameters
  - Population size, mutation rate, etc.
- Not much to say theoretically
  - Cross-over (sexual reproduction) much more efficient than mutation (asexual reproduction).
- Easy to implement
- Try hill-climbing with random restarts first!