Advanced Search

Hill climbing, simulated annealing, genetic algorithm

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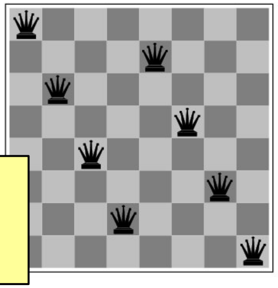
[Based on slides from Andrew Moore http://www.cs.cmu.edu/~awm/tutorials]

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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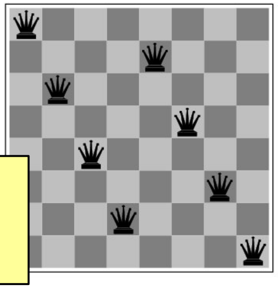

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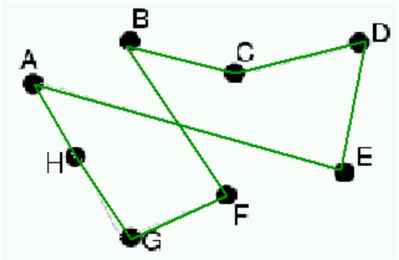
- Traveling salesperson problem (TSP)
  - Visit each city once, return to first city
  - State = order of cities, $f(s)$ = total mileage



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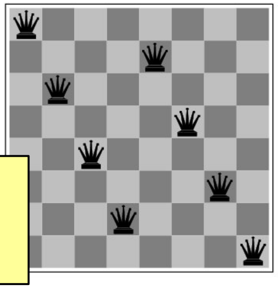

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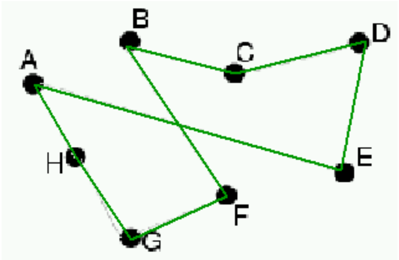

- Boolean satisfiability (e.g., 3-SAT)
  - State = assignment to variables
  - *f*(*s*) = # satisfied clauses

$A \vee \neg B \vee C$
$\neg A \vee C \vee D$
$B \vee D \vee \neg E$
$\neg C \vee \neg D \vee \neg E$
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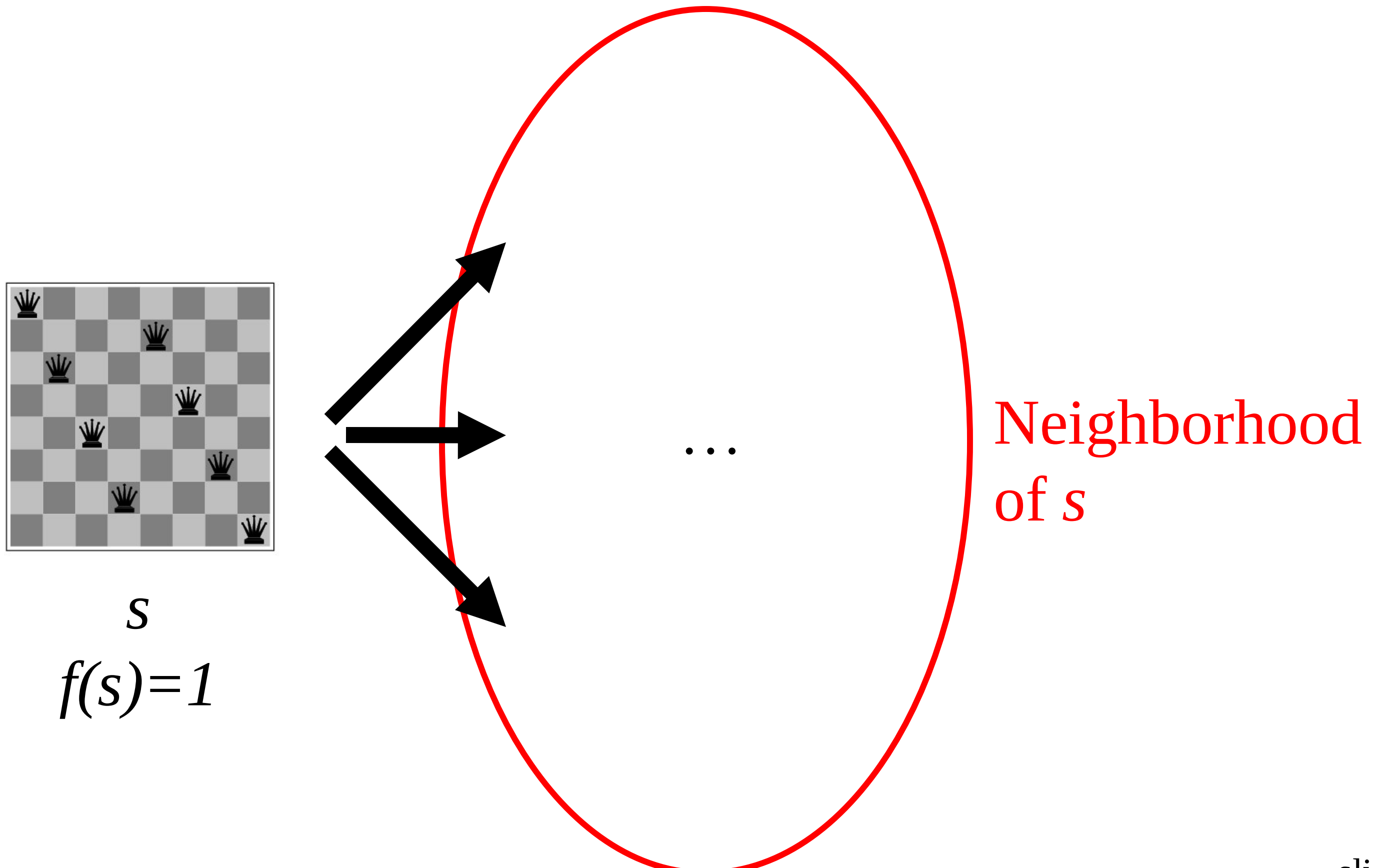
1. HILL CLIMBING

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

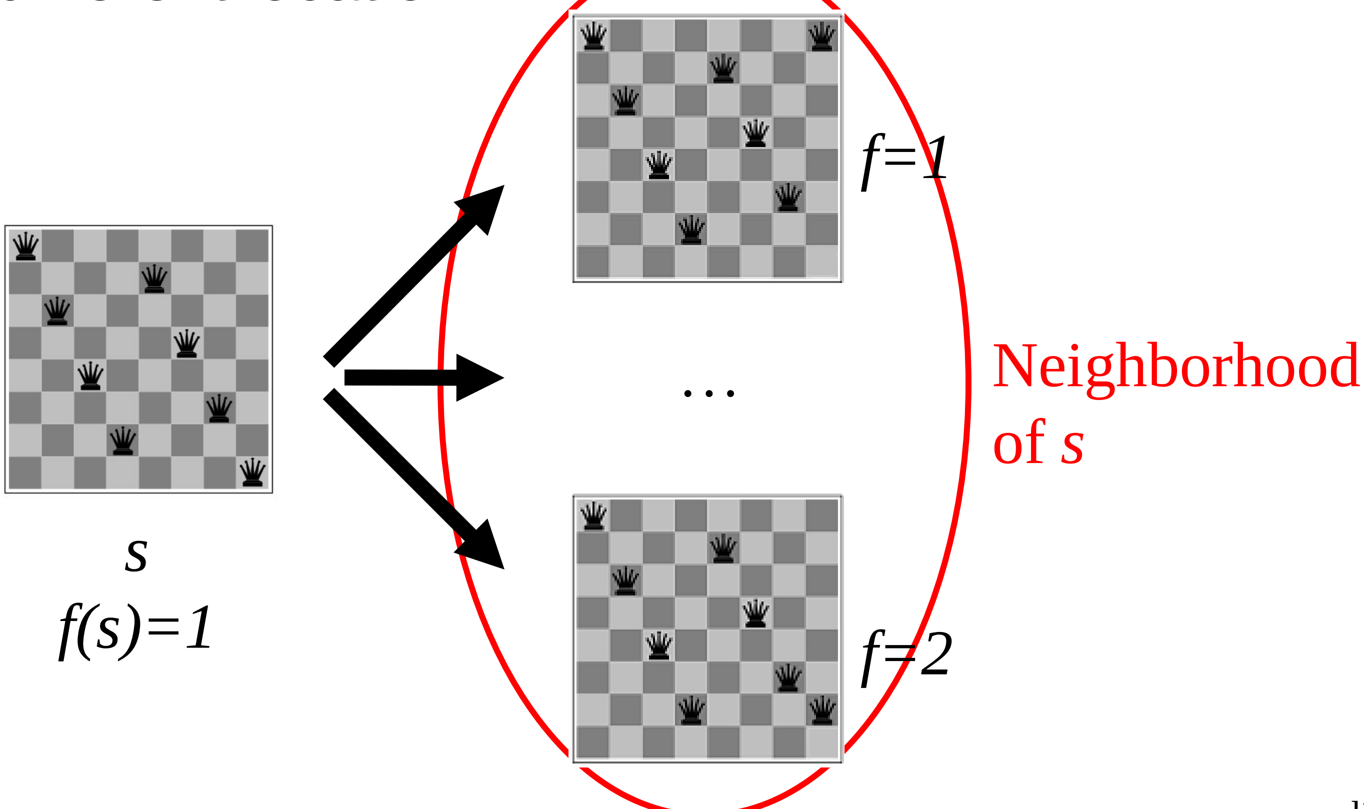
Neighbors: N-queen

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



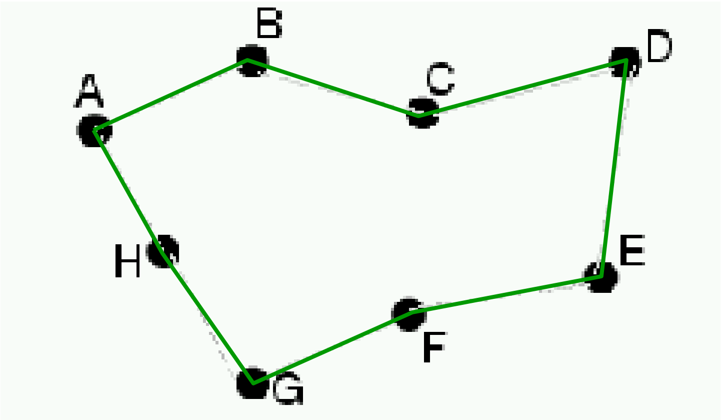
Neighbors: N-queen

- 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.



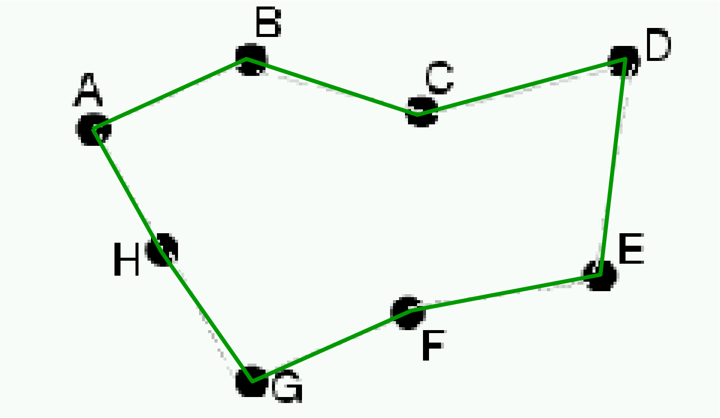
Neighbors: TSP

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



Neighbors: TSP

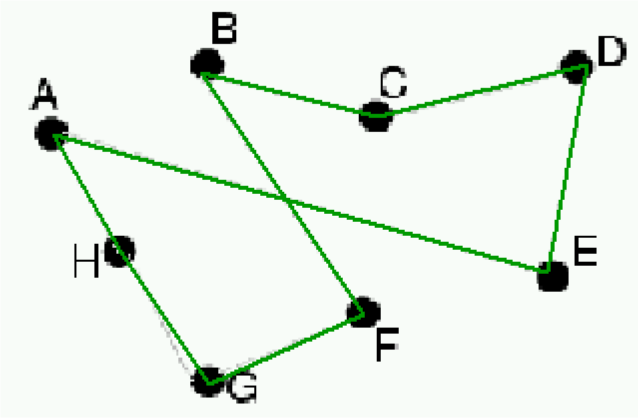
- state: A-B-C-D-E-F-G-H-A
- *f* = length of tour
- One possibility: 2-change



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:

$A \vee \neg B \vee C$
$\neg A \vee C \vee D$
$B \vee D \vee \neg E$
$\neg C \vee \neg D \vee \neg E$
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Neighbors: SAT

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

(A=**F**, B=F, C=T, D=T, 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?

Hill climbing

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  - (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? The best one (greedy)
- **Question**: What if no neighbor is better than the current state? Stop. (Doh!)

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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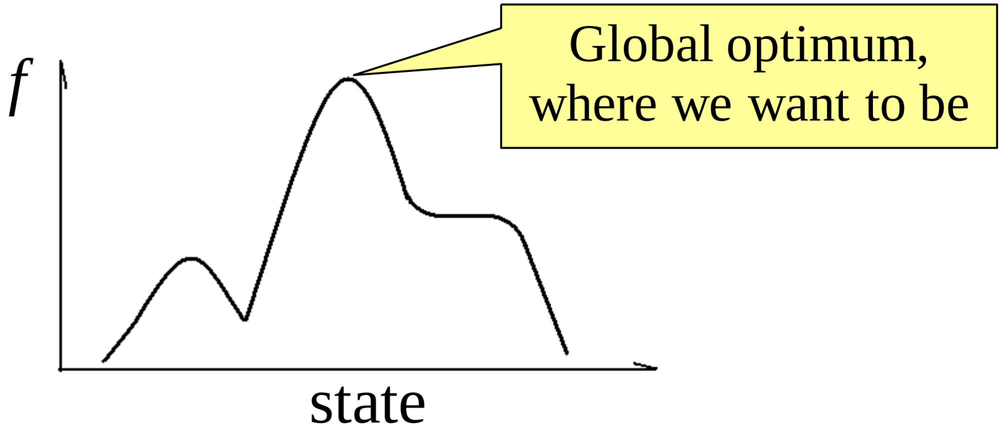
your enemy:

local

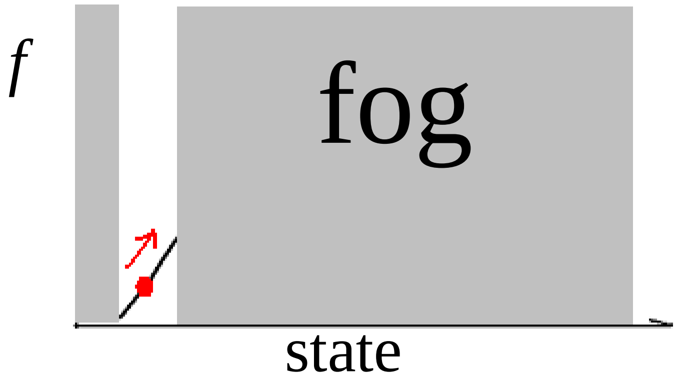
optima

Local optima in hill climbing

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

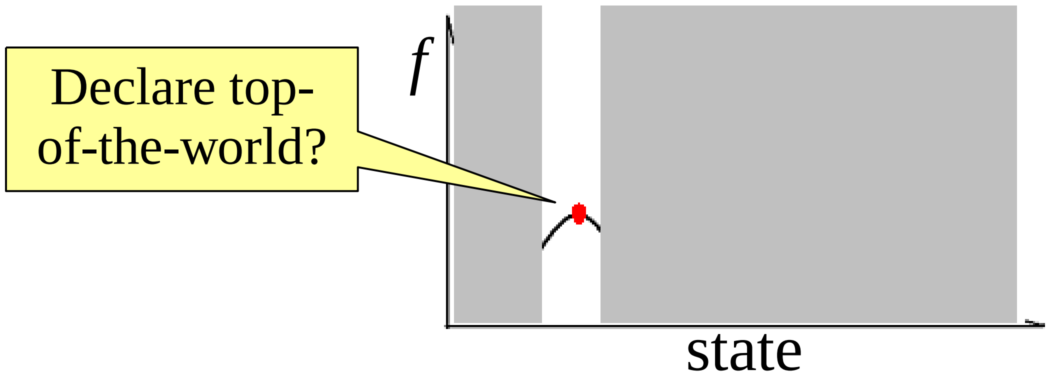


- But we can’t see the landscape all at once. Only see the neighborhood. Climb in fog.

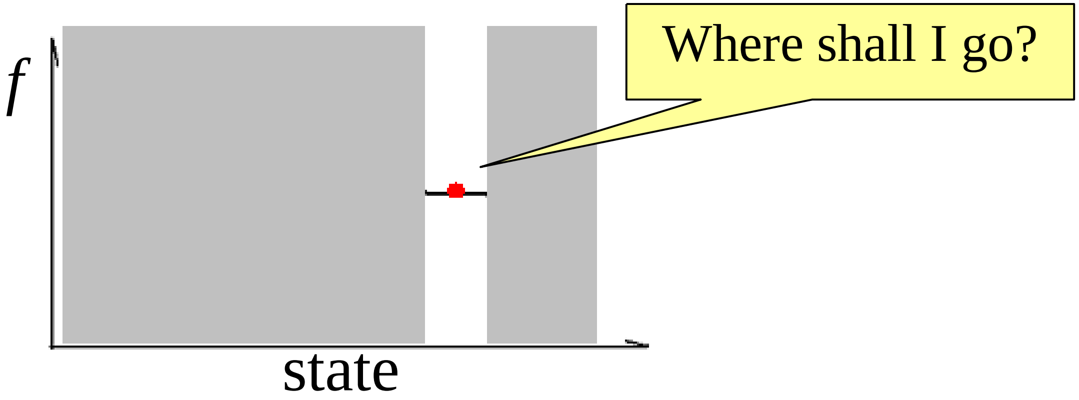


Local optima in hill climbing

- Local optima (there can be many!)



- Plateaux



Local optima in hill cl mbing

- Local optima (there ca e ma

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- Plate

ere shall I go?

e

The rest of the lecture is about

Escaping local optima

Not every local minimum should be escaped

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?

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Variations of hill climbing

- **Question**: How do we make hill climbing less greedy?
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    - The better, the more likely
    - Pros / cons compared with basic 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)
  - 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.

$A \vee \neg B \vee C$
$\neg A \vee C \vee D$
$B \vee D \vee \neg E$
$\neg C \vee \neg D \vee \neg E$
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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: $p = 0.1$

idea 2: p decreases with time

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.

SA 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

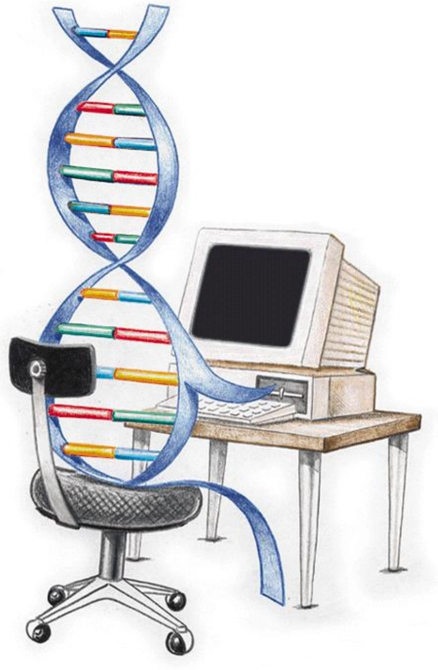
else current = next with probability p = exp(deltaE / T) ; // as T → 0, p → 0; as deltaE → -∞, p →0

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!

GENETIC ALGORITHM



http://www.genetic-programming.org/

Evolution

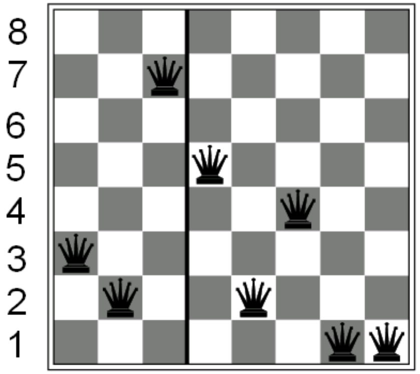
- Survival of the fittest, a.k.a. natural selection
- Genes encoded as DNA (deoxyribonucleic acid), sequence of bases: A (Adenine), C (Cytosine), T (Thymine) and G (Guanine)
- The chromosomes from the parents exchange randomly by a process called **crossover**. Therefore, the offspring exhibit some traits 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. from cosmic ray).
  - Nonsensical/deadly mutated organisms 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 lots of genes from the superior individuals, and less from the inferior individuals
- Superiority defined by fitness to the environment
- Popularized by Darwin
- Mistake of Lamarck: environment does not force an individual to change its genes

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

$A \lor \neg B \lor C$
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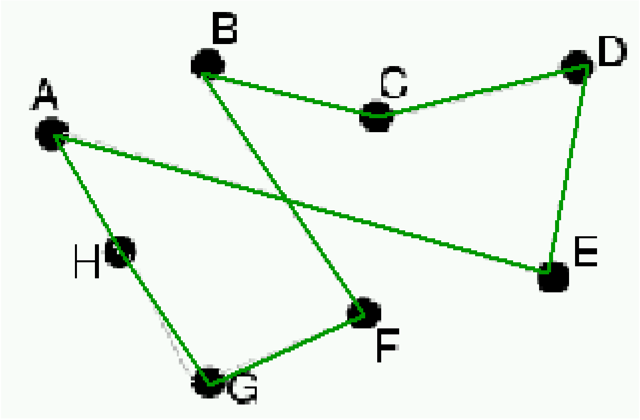
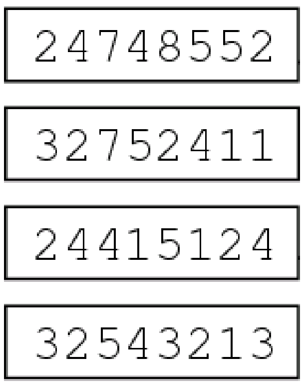


Genetic algorithm

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



(a)
Initial Population

Genetic algorithm

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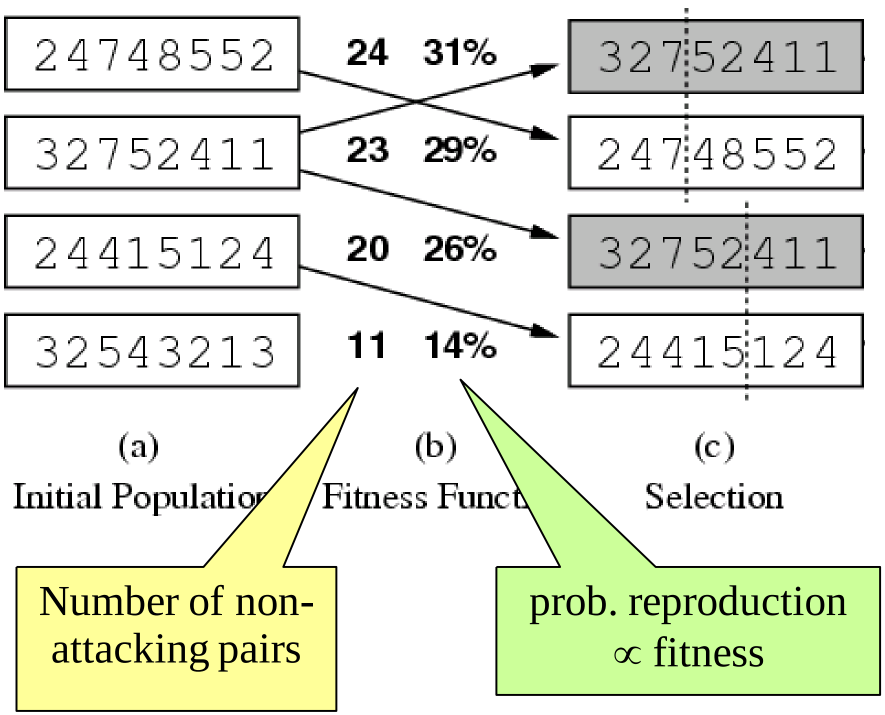

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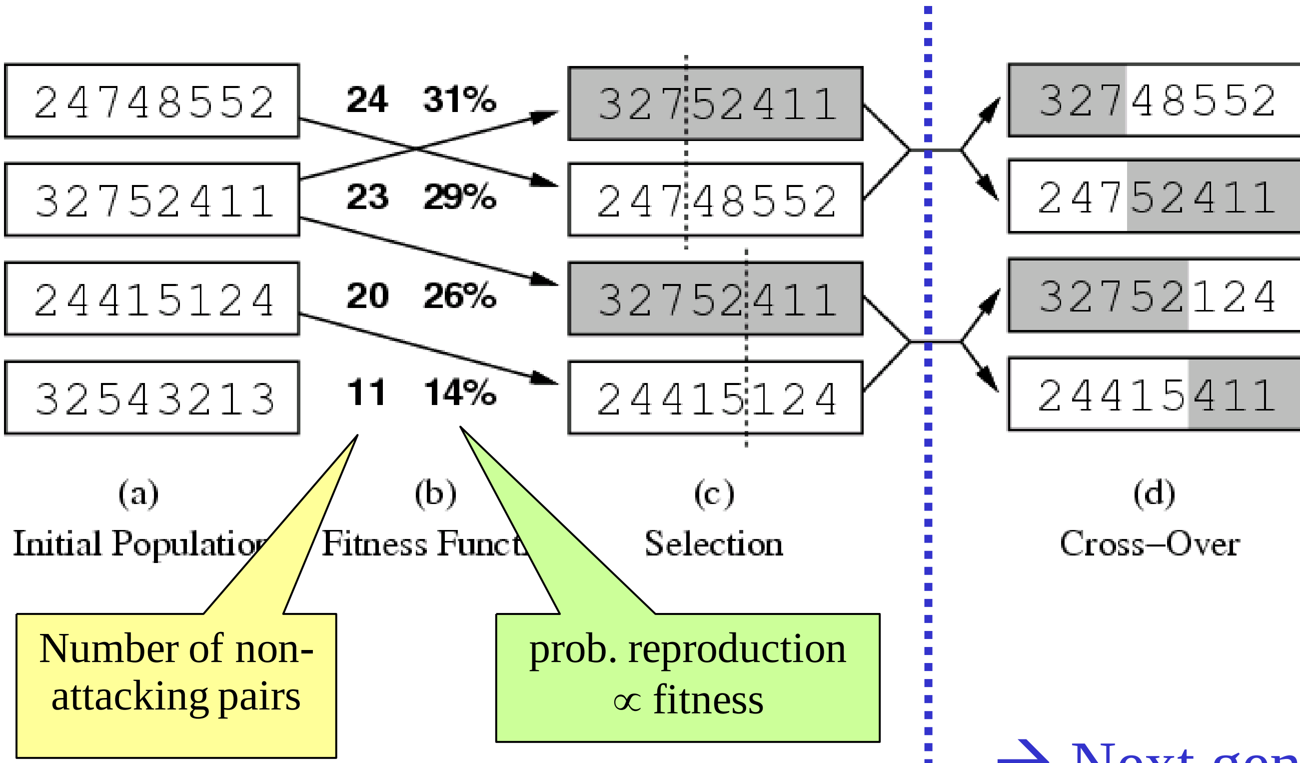

→ Next generation

Genetic algorithm

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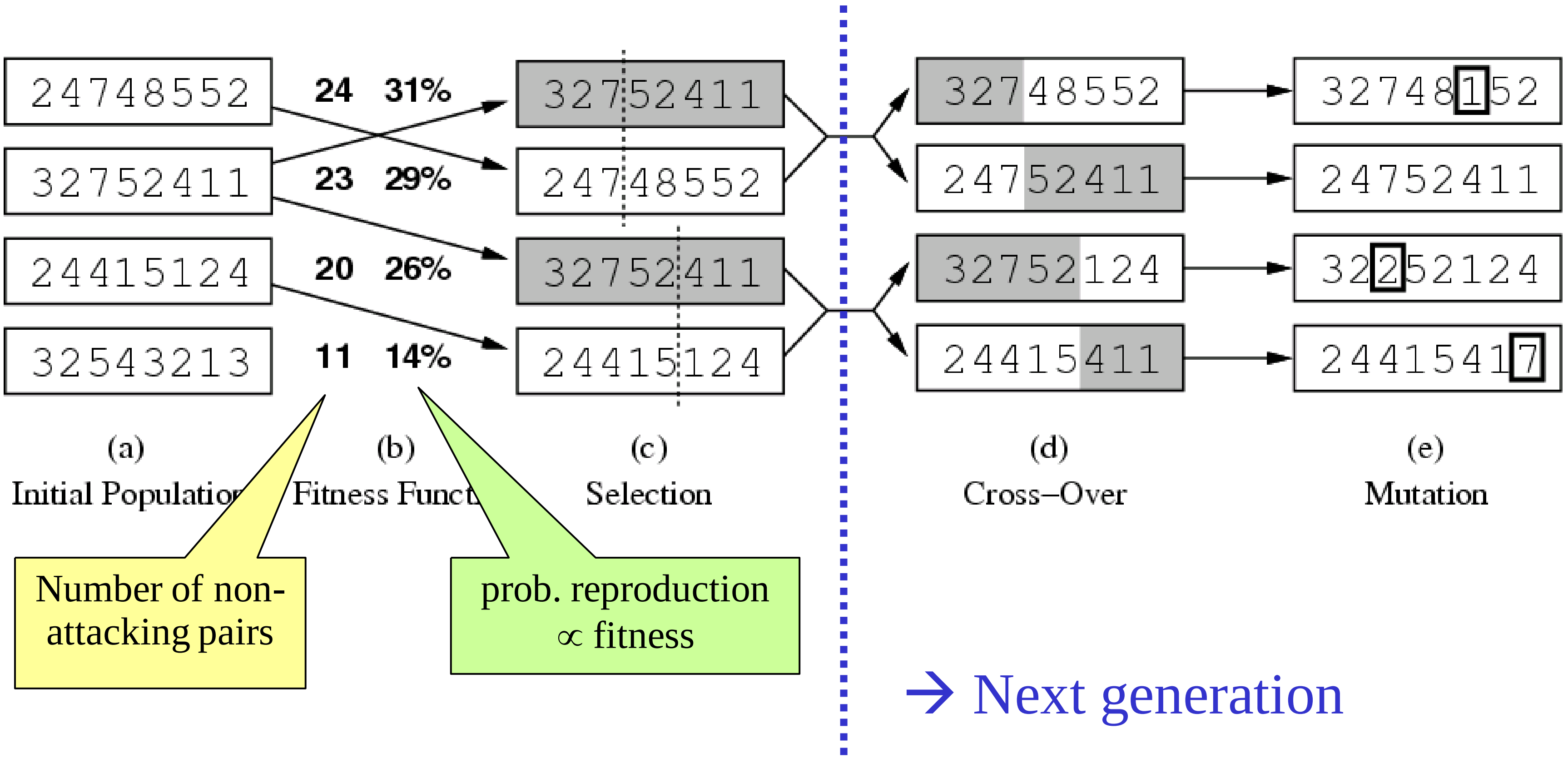

Genetic algorithm (one variety)

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.

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%

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
- 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!