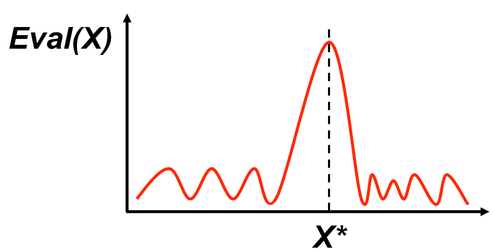
Lecture 4: Search for Optimization Problems

- What is an optimization problem?
- Local search algorithms:
  - Hill climbing
  - Simulated annealing

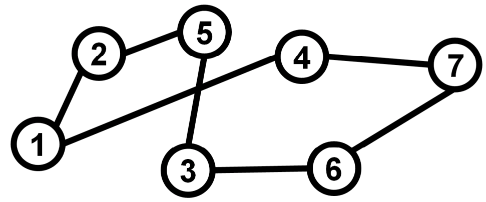
Optimization problems

- There is some combinatorial structure to the problem
- Constraints may have to be satisfied
- But there is also a *cost function*, which we want to optimize!



- Or at least, we want a "good" solution
- Searching all possible solutions is infeasible

Canonical example: Traveling Salesman Problem (TSP)



$X_1 = \{1\ 2\ 5\ 3\ 6\ 7\ 4\}$

- Given: a set of vertices and the distances between each pair of vertices
- Goal: construct the *shortest path that touches every vertex exactly once*
- A path that touches every vertex exactly once is called a tour.
- In the example above, X_1 is a tour, but not the optimal tour.

Real-life examples of optimization problems

- Scheduling
  - Given: a set of tasks to be completed, with durations and with mutual constraints (e.g. task ordering; joint resources)
  - Goal: generate the shortest schedule (assignment of start times to tasks) possible
- VLSI circuit layout
  - Given: a board, components and connections
  - Goal: place each component on the board such as to maximize energy efficiency, minimize production cost...
- In AI: learning, e.g.
  - Given: customers described by their characteristics (age, occupation, gender, location, etc) and their previous book purchases
  - Goal: find a function from customer characteristics to books which maximizes the probability of purchase

Characteristics of optimization problems

- Problem is described by a set of *states* (configurations) and an *evaluation function*

  E.g. in TSP, a tour is a state, and the length of the tour is the evaluation function (to minimize)
- The state space is too big to enumerate all states (or the evaluation may be expensive to compute for all states)

  E.g. in TSP, the state space is $(n-1)!/2$, where n is the number of vertices to connect
- We are only interested in the best solution, *not the path to the solution* (unlike in A^*)
- Often it is *easy* to find *some solution* to the problem
- Often it is provably *very hard* (NP-complete) to find the *best solution*

Types of search methods

1. *Constructive methods:* Start from scratch, build up a solution

   E.g. In TSP, start at the start city and add cities until a complete tour is formed
2. *Iterative improvement/repair methods:* Start with a solution (which may be "broken" or suboptimal) and improve it

   E.g. In TSP, start with a complete tour, and keep swapping cities to improve the cost

In both cases, the search is *local*: we have just one solution in mind, and we look for alternatives in the "vicinity" of that solution

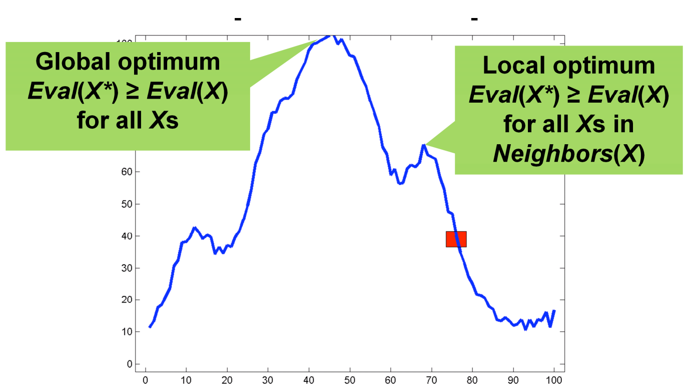
3. *Global search:* Start from multiple states that are far apart, and go all around the state space

Local search generic algorithm

1. Start from an initial configuration X_0
2. Repeat until *satisfied*:
   (a) Generate the *set of neighbors* of X_i and evaluate them
   (b) *Select* one of the neighbors, X_{i+1}
   (c) The selected neighbor becomes the current configuration

Choosing well the highlighted elements is crucial for a good algorithm!

Example



S = {1,…,100}

$Neighbors(X) = \{X-1, X+1\}$

How should we move around between solutions?

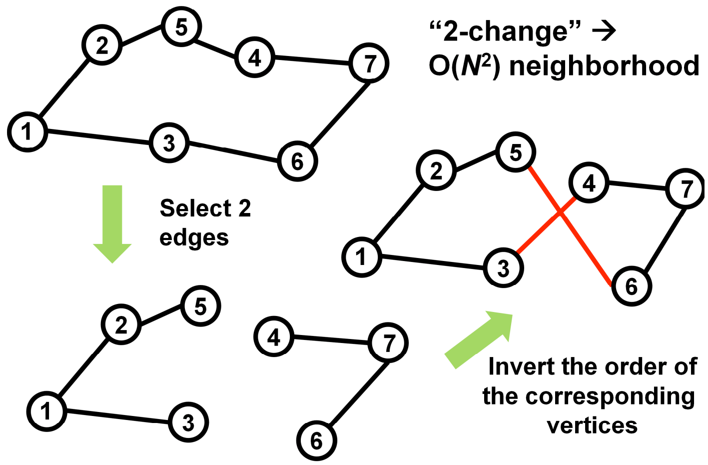
Hill climbing (greedy local search, gradient ascent/descent)

1. Start at initial configuration X and let E be the value of X (high is good)
2. Repeat
   (a) Let $X_i, i = 1 \ldots n$ be the set of neighboring configurations and E_i be the corresponding values
   (b) Let $E_{max} = \max_i E_i$ be the value of the best successor configuration and $i_{max} = \arg\max_i E_i$ be the index of the best configuration.
   (c) If $E_{max} \leq E$, return X (we are at a local optimum)
   (d) Else let $X \leftarrow X_{i_{max}}$ and $E \leftarrow E_{max}$

Good things about hill climbing

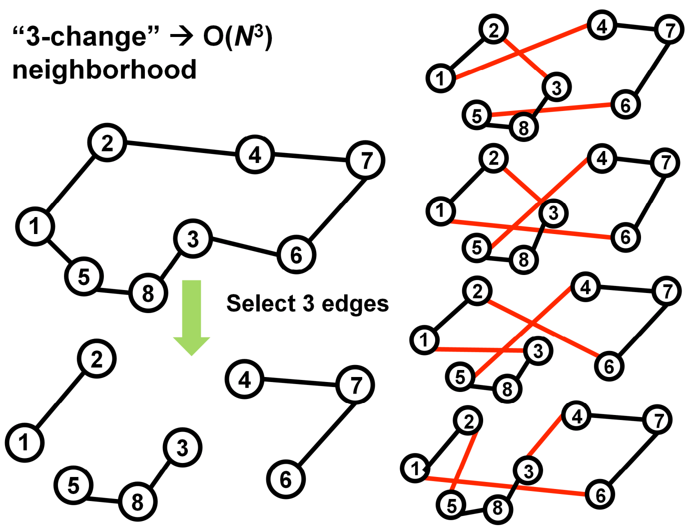
- Trivial to program!
- Requires no memory of where we've been (because it does no backtracking)
- It is important to have a "good" set of neighbors (not too many, not too few)

Example: TSP, swapping two nodes



$O(n^2)$ comes from the fact that we have n edges in a tour, and choose two of them to swap, so there are $\binom{n}{2}$ possible next tours

Example: TSP, swapping three nodes



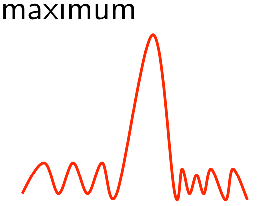
There are $\binom{n}{3}$ combinations of edges to choose, and for each set of edges, more than one possible neighbor

Neighborhood trade-off

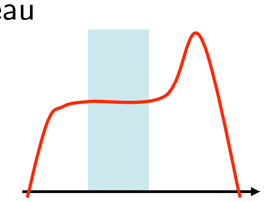
- A smaller neighborhood means fewer neighbors to evaluate (so cheaper computation, but possibly worse solutions)
- A bigger neighborhood means more computation, but maybe fewer local optima, so better final result
- Defining the set of neighbors is a *design choice* (like choosing the heuristic for A^*) and has a crucial impact on performance
- For realistic problems, there may not be a unique way of defining the neighbors

Problems with hill climbing

- Can get stuck in a local maximum



- Can get stuck on a plateau

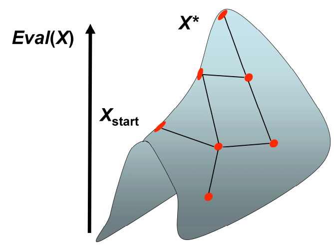


- Relies very heavily on having a good neighborhood function and a good evaluation function, in order to get an easy-to-navigate "solution landscape"

Improvements to hill climbing

- Quick fix: when stuck in a plateau or local optimum, use *random restarts*
- Better fix: Instead of picking the best move pick *any move that produces an improvement*

  This is called *randomized hill climbing*
- But sometimes we may really need to pick apparently bad moves!

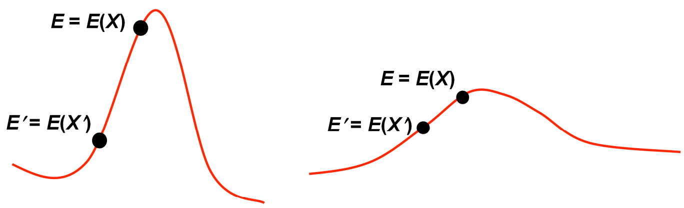


E.g. Assuming salary is the evaluation function, you can pick a dead-end job but which pays well right away, vs. picking a job that pays less now, but you learn skills that may lead to a better job later

Simulated annealing

- Allows some apparently *"bad moves"*, in the hope of escaping local maxima
- Decrease the size and frequency of "bad moves" over time
- Algorithm sketch
  1. Start at initial configuration X of value E (high is good)
  2. Repeat:
     (a) Let X_i be a *random neighbor* of X and E_i be its value
     (b) If $E < E_i$ then let $X \leftarrow X_i$ and $E \leftarrow E_i$
     (c) Else, *with some probability* p, still accept the move: $X \leftarrow X_i$ and $E \leftarrow E_i$
- Best solution ever found is always remembered

What value should we use for p?



- Suppose you are at a state of value E and are considering a move to a state of lower value E'
- If $E - E'$ is large, you are likely close to a promising maximum, so you should be less likely to want to go downhill
- If $E - E'$ is small, the closest maximum may be shallow, so going downhill is not as bad
- We may want different neighbors with similar value to be equally likely to be picked
- As we get more experience with the problem, we may want to settle on the solution (landscape has been explored enough)

Selecting moves in simulated annealing

- If the new value E_i is better than the old value E, move to X_i
- If the new value is worse $(E_i < E)$ then move to the neighboring solution with probability:
$$\exp\left(-\frac{E - E_i}{T}\right)$$
This is called the *Boltzmann distribution*
- $T > 0$ is a parameter called *temperature*, which typically starts high, then decreases over time towards 0
- If T is high, exponent is close to 0 and probability of accepting any move is close to 1
- If T is very close to 0, the probability of moving to a worse solution is almost 0.
- We can decrease T by multiplying with a constant $\alpha < 1$ on every move (or some other, fancier "schedule")

Where does the Boltzmann distribution come from?

- For a solid, at temperature T, the probability of moving between two states of energy difference ΔE is:

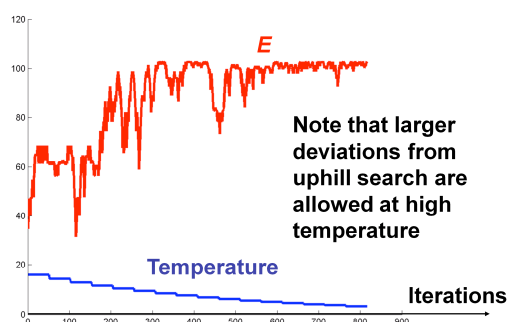
$$e^{-\Delta E/kT}$$

- If temperature decreases slowly, it will reach an equilibrium, at which the probability of being in a state of energy E is proportional to:

$$e^{-E/kT}$$

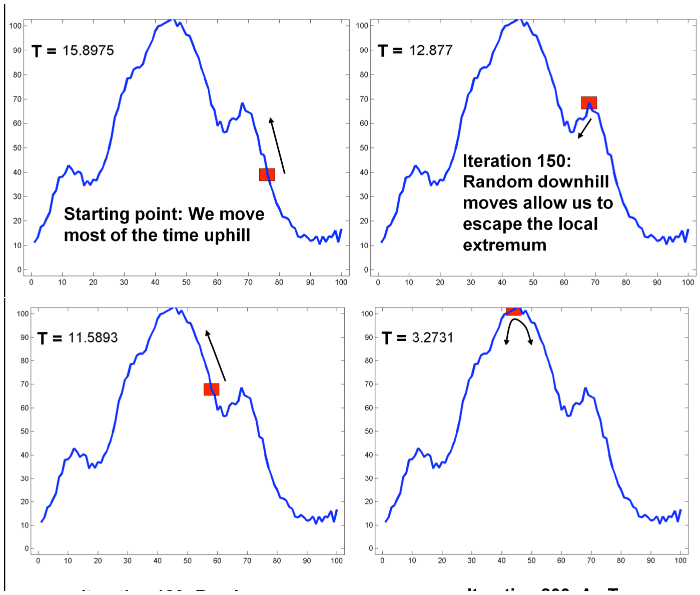
- So states of low energy (relative to T) are more likely
- In our case, states with better value will be more likely

Properties of simulated annealing

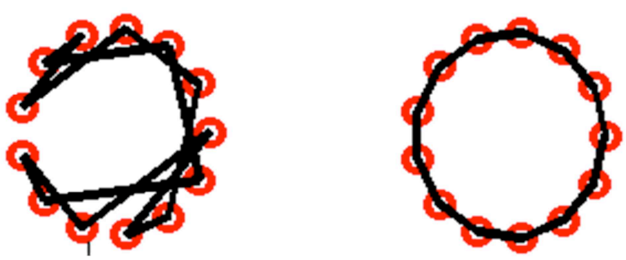


- When T is high, the algorithm is in an *exploratory phase* (even bad moves have a high chance of being picked)
- When T is low, the algorithm is in an *exploitation phase* (the "bad" moves have very low probability
- If T is decreased slowly enough, simulated annealing is guaranteed to reach the best solution *in the limit* (but there is no guarantee how fast...)

Example



TSP example



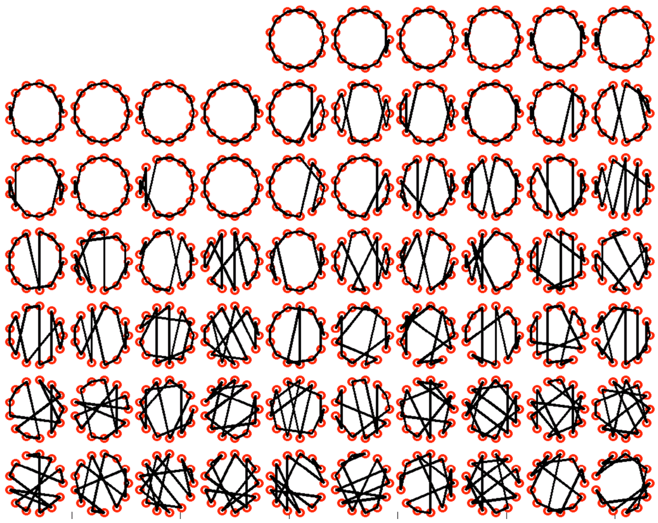
N = 13 nodes (in a circle)

Repeat K = 100N times

Optimal configuration has E = 25

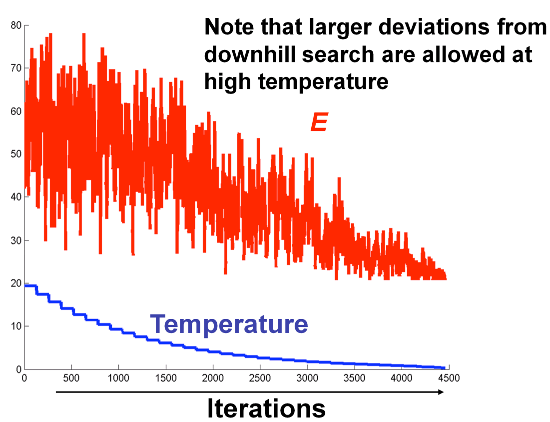
Starting configuration has E = 55

TSP example: Configurations



The initial configuration is bottom right, final one is top left

TSP example: Energy



Simulated annealing in practice

- Very useful algorithm, used to solve very hard optimization problems:
  - E.g. What gene network configuration best explains observed expression data
  - E.g. Scheduling large transportation fleets
- The *temperature annealing schedule is crucial* (so it needs to be tweaked)
  - Cool too fast and you do not reach optimality
  - Slow cooling leads to very slow improvements
- On large problems, simulated annealing can take days or weeks
- Simulated annealing is an example of a *randomized search* or *Monte Carlo search*
- Basic idea: run around through the environment and explore it, instead of systematically sweeping
- *Very powerful for large domains!*

Summary

- Optimization problems are widespread and important
- We are only interested in the final result, rather than the path to it
- It is unfeasible to enumerate all possible solutions
- Instead we can do a *local search* and move in the most promising direction:
  - *Hill climbing* (a.k.a. gradient ascent/descent) always moves in the (locally) best direction
  - *Simulated annealing* allows moves downhill
- Next time: *global search*, looking for solutions from multiple points in parallel
  - *Genetic algorithms* use an evolutionary-inspired procedure
  - Ant-colony optimization and other methods are also possible.
- Important lesson: *the power of randomness!*
  This is a key ingredient for escaping local optima