CS 1571 Introduction to AI
Lecture 8

Methods for finding optimal configurations

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Announcements

- **Homework assignment 2 due today**
- **Homework assignment 3 is out**
  – Programming and experiments
  – Simulated annealing + Genetic algorithm
  – Competition

Course web page:

http://www.cs.pitt.edu/~milos/courses/cs1571/

Search for the optimal configuration

Optimal configuration search:

- Configurations are described in terms of variables and their values
- Each configuration has a quality measure
- **Goal:** find the configuration with the best value

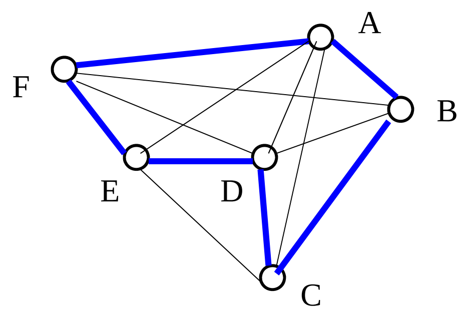
If the space of configurations we search among is

- **Discrete or finite**
  - **then it is a combinatorial optimization problem**
- **Continuous**
  - **then it is a parametric optimization problem**

Example: Traveling salesman problem

Problem:

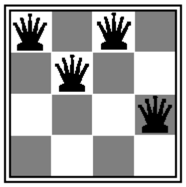
- A graph with distances
- A tour – a path that visits every city once and returns to the start e.g. ABCDEF



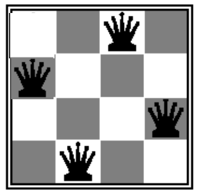
- **Goal:** find the shortest tour

Example: N queens

- Originally a CSP problem
- But it is also possible to formulate the problem as an optimal configuration search problem:
- **Constraints are mapped to the objective cost function that** counts the number of violated constraints



# of violations =3



# of violations =0

Iterative optimization methods

- Searching systematically for the best configuration with the **DFS** may not be the best solution
- Worst case running time:
  - Exponential in the number of variables
- Solutions to **large 'optimal' configuration** problems are often found more effectively in practice using iterative optimization methods

- **Examples of Methods:**
  - **Hill climbing**
  - **Simulated Annealing**
  - **Genetic algorithms**

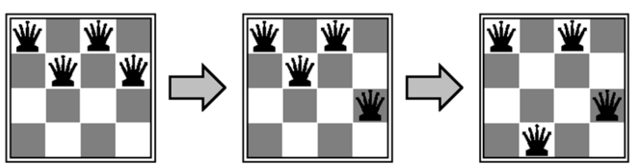
Iterative optimization methods

Basic Properties:

- **Search the space of "complete" configurations**
- **Take advantage of local moves**
  - Operators make "local" changes to "complete" configurations
- **Keep track of just one state (the current state)**
  - no memory of past states
  - **!!! No search tree is necessary !!!**

Example: N-queens

- **"Local" operators for generating the next state:**
  - Select a variable (a queen)
  - Reallocate its position



Example: Traveling salesman problem

"Local" operator:

– generates the next configuration (state) by rearranging the existing tour

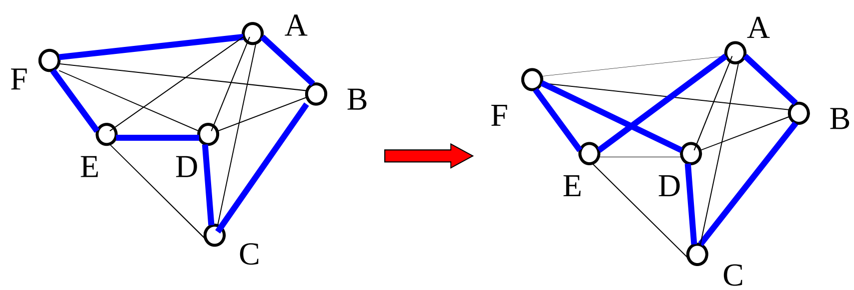
ABCDEF

↓

ABCD | EF |

↓

ABCDFE



Search algorithms

Strategies to choose the configuration (state) to be visited next:

- **Hill climbing**
- **Simulated annealing**

• Extensions to multiple current states:

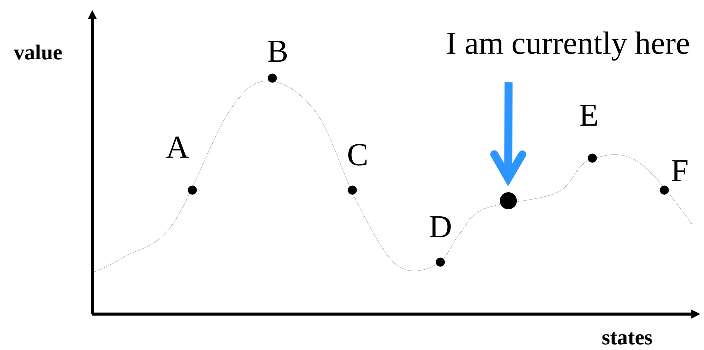
- **Genetic algorithms**
- **Beam search**

• **Note:** Maximization is inverse of the minimization

$$\min f(X) \Leftrightarrow \max\left[-f(X)\right]$$

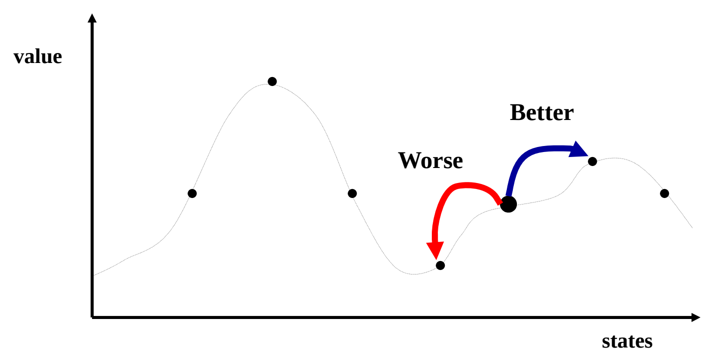
Hill climbing

- What configurations are considered next?
- What move the hill climbing makes?



Hill climbing

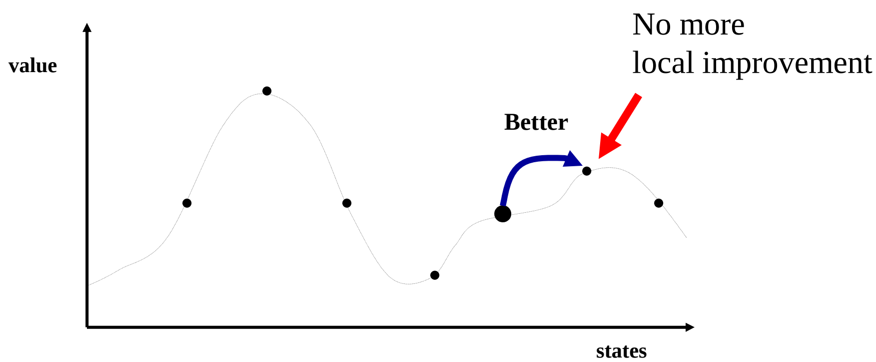
- Look at the local neighborhood and choose the one with the best value



- **What can go wrong?**

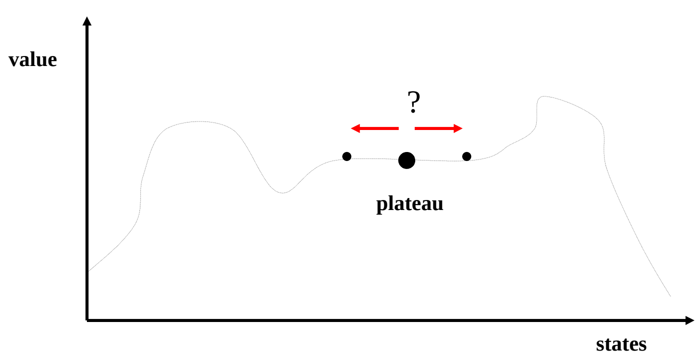
Hill climbing

- Hill climbing can get trapped in the local optimum



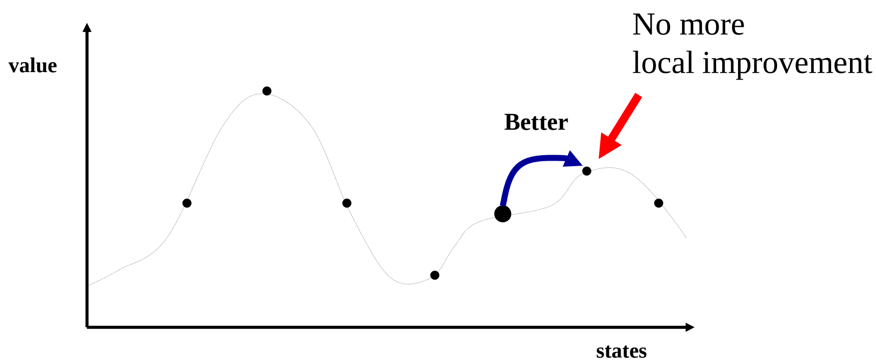
Hill climbing

- Hill climbing can get clueless on plateaus



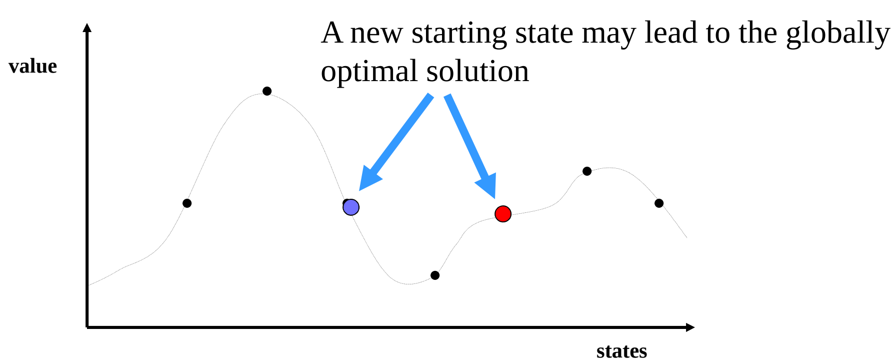
Hill climbing

- **How to remedy the problem of local optima?**



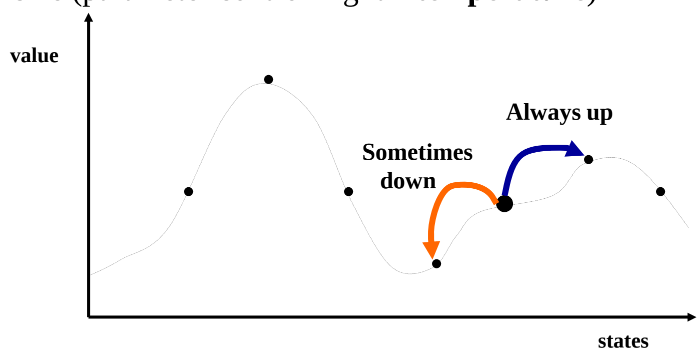
Hill climbing

- **Multiple restarts** of the hill climbing algorithms from different initial states



Simulated annealing

- An alternative solution to the local optima problem
- Permits “bad” moves to states with a lower value hence lets us escape states that lead to a local optima
- **Gradually decreases** the frequency of such moves and their size (parameter controlling it – **temperature**)



Simulated annealing algorithm

- **Based on a random walk in the configuration space**

Basic iteration step:

- Choose uniformly at random one of the local neighbors of the current state as a candidate state
- **if** the candidate state is better than the current state

  then

  accept the candidate and make it the current state;

  else

  calculate the probability p(ACCEPT) of accepting it

  using p(ACCEPT) choose randomly whether to accept

  or reject the candidate

Simulated annealing algorithm

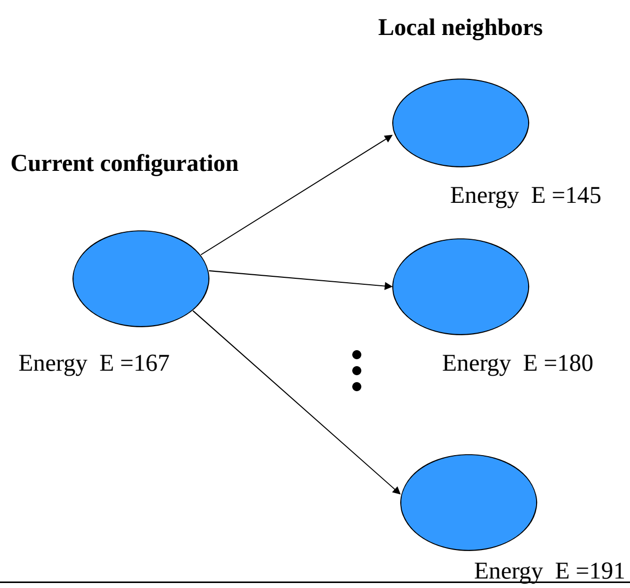
The probability p(ACCEPT) of the candidate state:

- The probability of accepting a state with a better objective function value is 1
- The probability of accepting a candidate with a lower objective function value is < 1 and equal:
- Let E denotes the objective function value (also called energy).

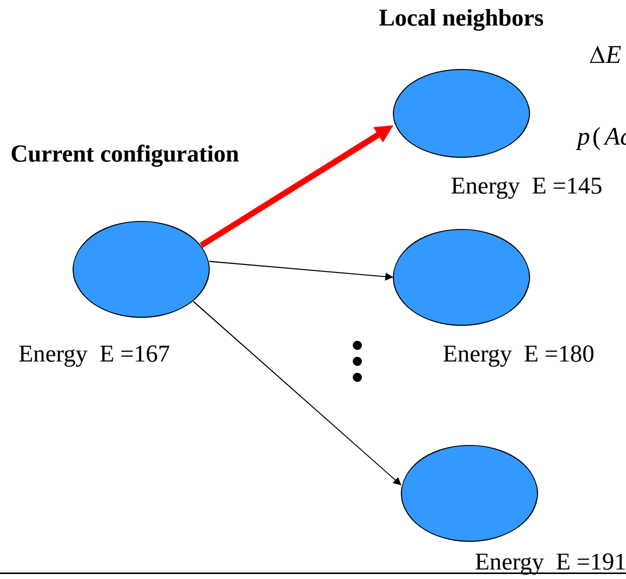
$$p(Accept\ NEXT) = e^{\Delta E / T} \quad \text{where} \quad \Delta E = E_{NEXT} - E_{CURRENT}, \quad T > 0$$

- The probability is:
  - **Proportional to the energy difference**

Simulated annealing algorithm



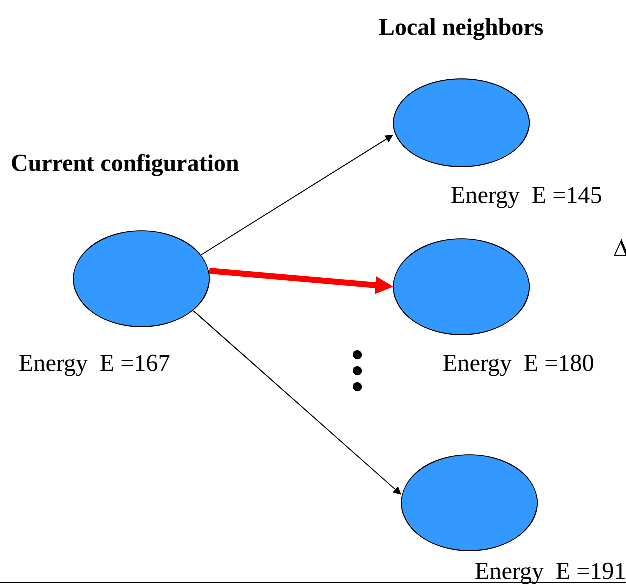
Simulated annealing algorithm



$$\Delta E = E_{NEXT} - E_{CURRENT}$$
$$= 145 – 167 = -22$$
$$p(Accept) = e^{\Delta E / T} = e^{-22/T}$$

Sometimes accept!

Simulated annealing algorithm



$$\Delta E = E_{NEXT} - E_{CURRENT}$$
$$= 180 – 167 > 0$$
$$p(Accept) = 1$$

Always accept!

Simulated annealing algorithm

The probability of accepting a state with a lower value is

$$p(Accept) = e^{\Delta E / T} \quad \text{where} \quad \Delta E = E_{NEXT} - E_{CURRENT}$$

The probability is:

- **Modulated through a temperature parameter T**:
  - for $T \to \infty$ the probability of any move approaches 1
  - for $T \to 0$ the probability that a state with smaller value is selected goes down and approaches 0
- **Cooling schedule:**
  - Schedule of changes of a parameter T over iteration steps

Simulated annealing algorithm

The probability of accepting a state with a lower value is

$$p(Accept) = e^{\Delta E / T} \quad \text{where} \quad \Delta E = E_{NEXT} - E_{CURRENT}$$

The probability p(accept) is:

- **Modulated through a temperature parameter T**:
  - for $T \to \infty$?
  - for $T \to 0$?
- **Cooling schedule:**
  - Schedule of changes of a parameter T over iteration steps

Simulated annealing algorithm

The probability of accepting a state with a lower value is

$p(Accept) = e^{\Delta E / T}$ where $\Delta E = E_{NEXT} - E_{CURRENT}$

The probability is:

- **Modulated through a temperature parameter T**:
  - for $T \rightarrow \infty$ the probability of any move approaches 1
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- **Cooling schedule:**
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Simulated annealing

function SIMULATED-ANNEALING(*problem*, *schedule*) **returns** a solution state
  inputs: *problem*, a problem
      schedule, a mapping from time to "temperature"
  static: *current*, a node
      next, a node
      T, a "temperature" controlling the probability of downward steps

  current ← MAKE-NODE(INITIAL-STATE[*problem*])
  for *t* ← 1 **to** ∞ **do**
    T ← *schedule*[*t*]
    if *T*=0 **then return** *current*
    next ← a randomly selected successor of *current*
    ΔE ← VALUE[*next*] – VALUE[*current*]
    if $\Delta E > 0$ **then** *current* ← *next*
    else *current* ← *next* only with probability $e^{\Delta E/T}$

Simulated annealing algorithm

- **Simulated annealing algorithm**
  - developed originally for modeling physical processes (Metropolis et al, 53)
- **Properties:**
  - **If temperature T is decreased slowly enough the best configuration (state) is always reached**
- **Applications:**
  - VLSI design
  - airline scheduling

Simulated evolution and genetic algorithms

- Limitations of **simulated annealing**:
  - Pursues one state configuration at the time;
  - Changes to configurations are typically local

Can we do better?

- Assume we have two configurations with good values that are quite different
- We expect that the combination of the two individual configurations may lead to a configuration with higher value

(**Not guaranteed !!!)**

This is the idea behind **genetic algorithms** in which we grow a population of candidate solutions generated from combination of previous configuration candidates

Genetic algorithms

Algorithm idea:

- **Create a population of random configurations**
- **Create a new population through:**
  - Biased selection of pairs of configurations from the previous population
  - Crossover (combination) of selected pairs
  - Mutation of resulting individuals
- **Evolve the population over multiple generation cycles**

- **Selection of configurations to be combined:**
  - **Fitness function = value of the objective function**

    measures the quality of an individual (a state) in the population

Reproduction process in GA

- Assume that a state configuration is defined by a set variables with two values, represented as 0 or 1