## CS 1571 Introduction to AI
## Lecture 9

# Methods for finding optimal configurations

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## Search for the optimal configuration

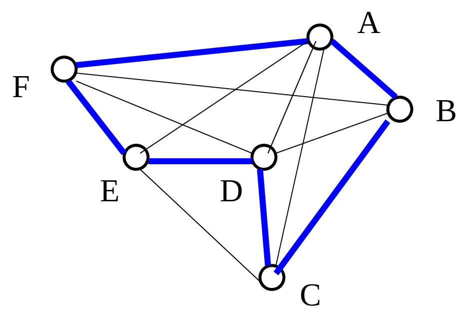
**Optimal configuration search:**
- Configurations are described in terms of variables and their values
- Each configuration has a quality measure
- **Goal:** find the configuration with the best value

**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

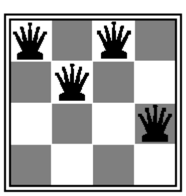



- **Goal:** find the shortest tour

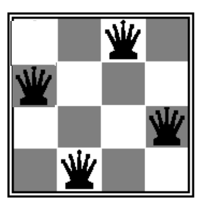


## Example: N queens

- 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



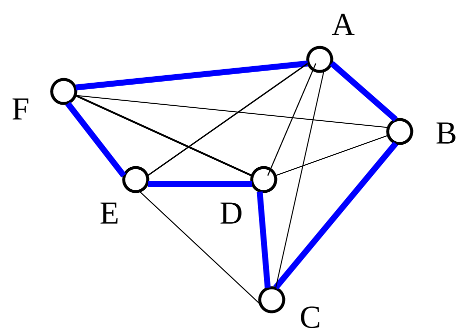
# Example: Traveling salesman problem

**“Local” operator for generating the next state:**

- divide the existing tour into two parts,
- reconnect the two parts in the opposite order

**Example:**

ABCDEF



# Example: Traveling salesman problem

**"Local" operator for generating the next state:**

- divide the existing tour into two parts,
- reconnect the two parts in the opposite order

**Example:**

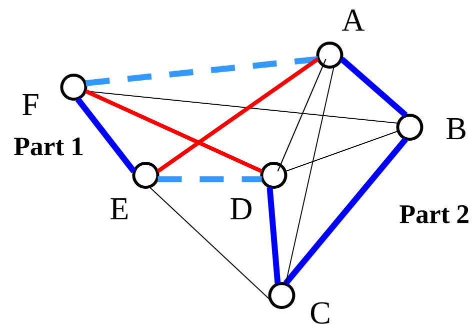
ABCDEF

⇓

ABCD | EF |

⇓

ABCDFE

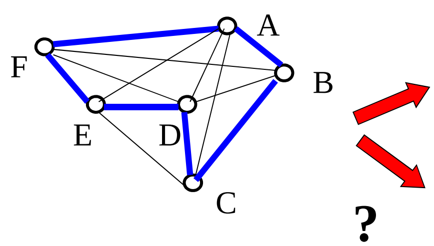


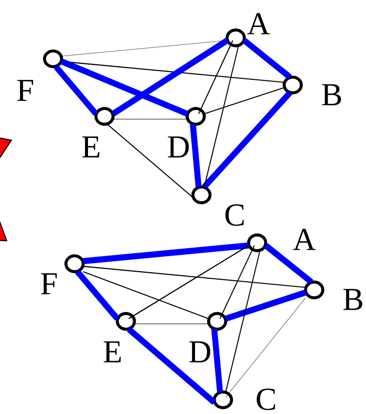



# Searching the configuration space

**Search algorithms**

- keep only one configuration (the current configuration)




**Problem:**

- How to decide about which operator to apply?

## Search algorithms

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

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

- **Later:** Extensions to multiple current states:
  - **Genetic algorithms**

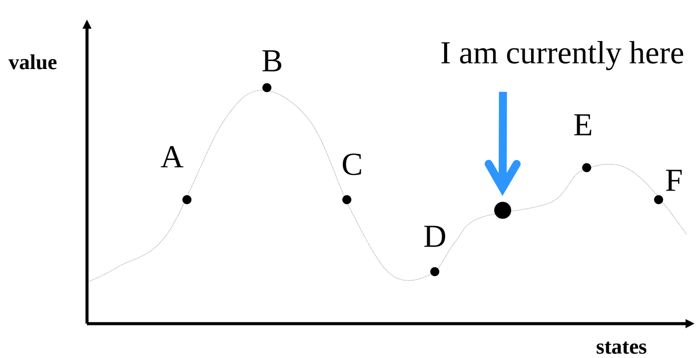
- **Note:** Maximization is inverse of the minimization

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



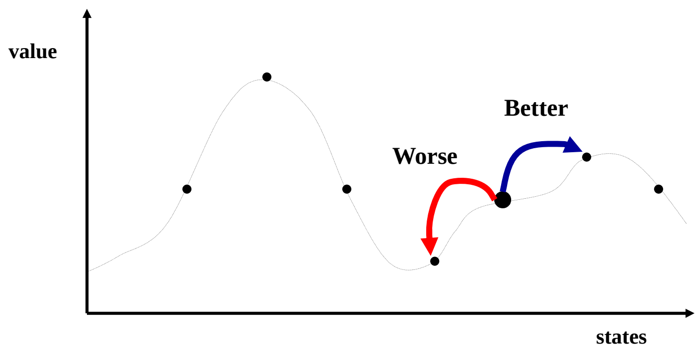
## Hill climbing

- Only configurations one can reach using local moves are consired as candidates
- What move the hill climbing makes?



## Hill climbing

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

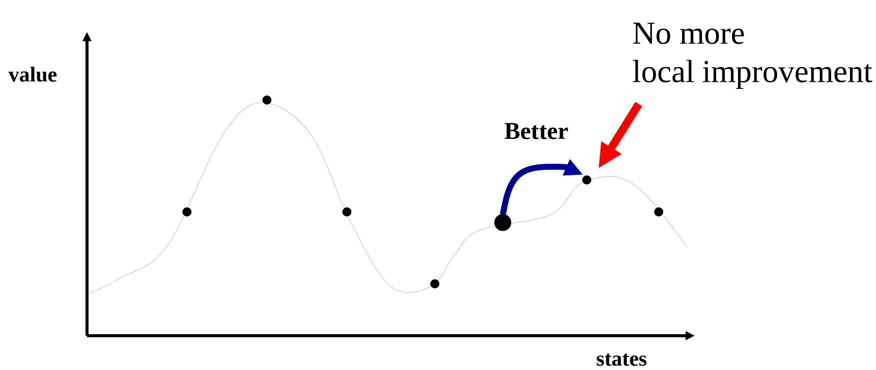



- **What can go wrong?**



## Hill climbing

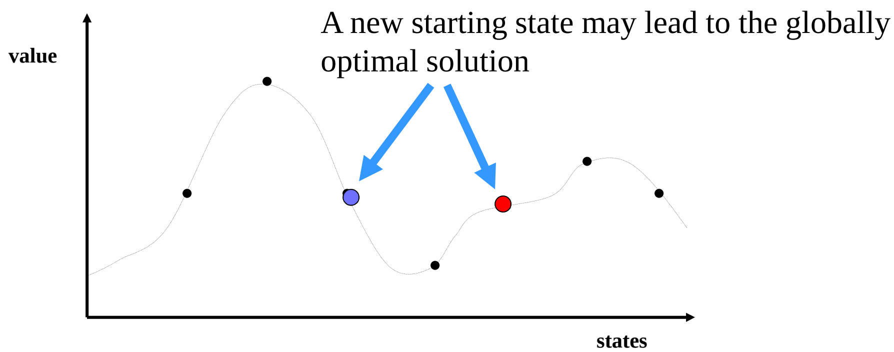
- Hill climbing can get trapped in the local optimum




- **How to solve the problem? Ideas?**

# Hill climbing

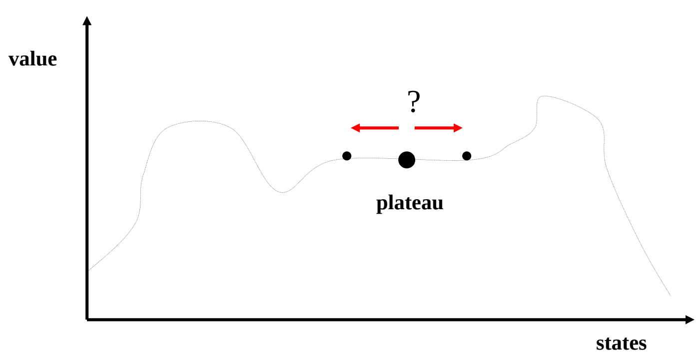
- **Solution: Multiple restarts** of the hill climbing algorithms from different initial states





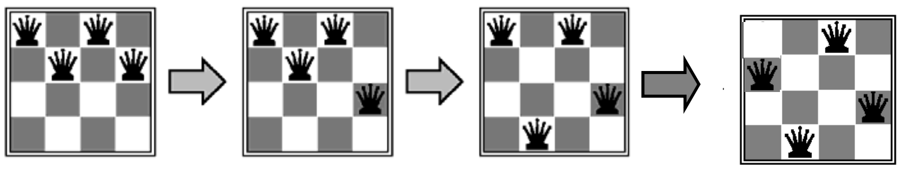

# Hill climbing

- Hill climbing can get clueless on plateaus



## Hill climbing and n-queens

- The quality of a configuration is given by the number of constraints violated
- **Then: Hill climbing** reduces the number of constraints
- **Min-conflict strategy (heuristic):**
  - Choose randomly a variable with conflicts
  - Choose its value such that it violates the fewest constraints

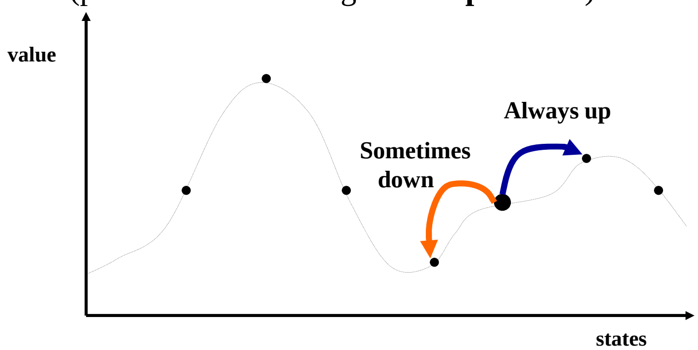


Success !! But not always!!! The local optima problem!!!



## 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

**end**



## Simulated annealing algorithm

**The probability p(ACCEPT) of the candidate state:**

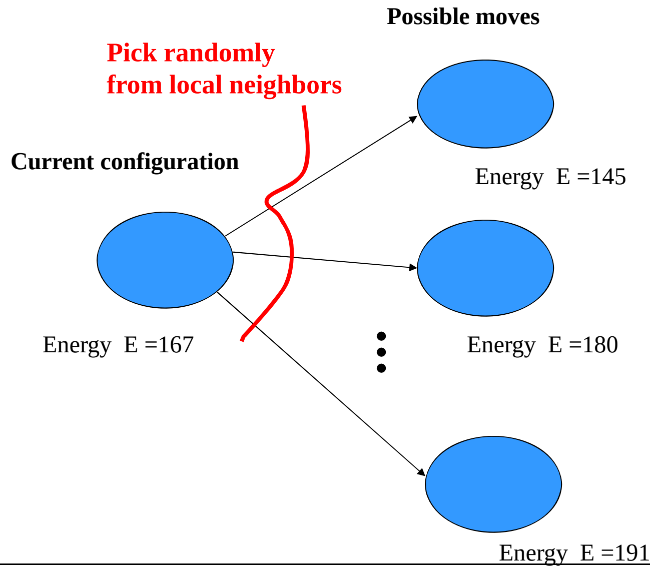
- The probability of accepting a state with a better objective function value is **always 1**
- The probability of accepting a candidate with a lower objective function value is < 1 and equal:
- Let E denotes the objective function value (also called energy).

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

where
$$\Delta E = E_{NEXT} - E_{CURRENT}$$
$$T > 0$$

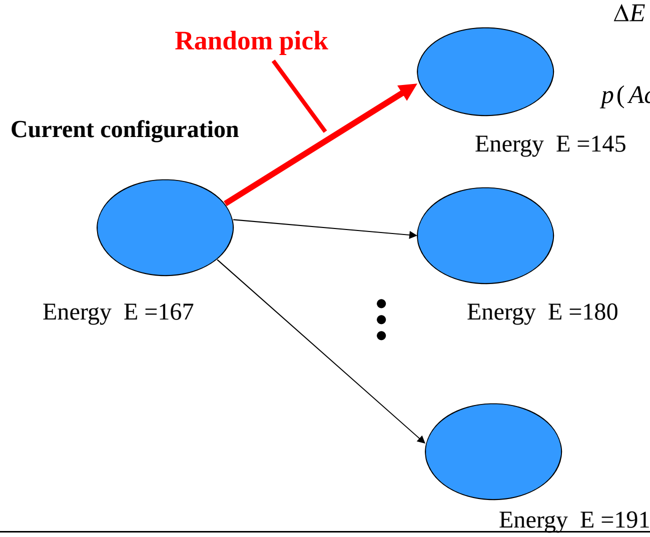
- The probability is:
  - **Proportional to the energy difference**

# Simulated annealing algorithm





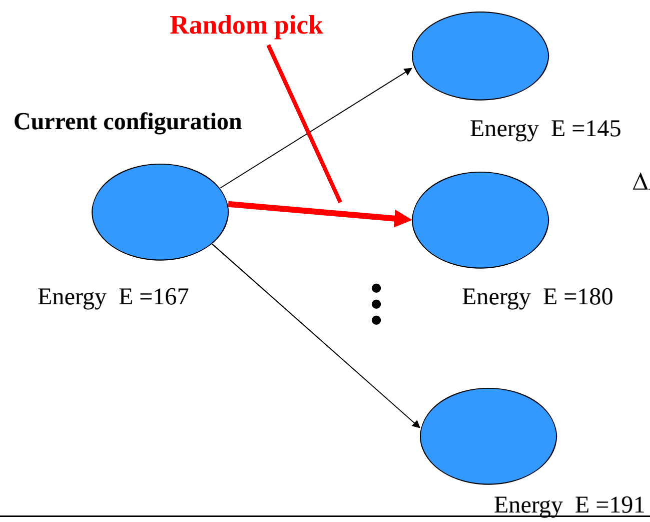

# Simulated annealing algorithm




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

**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 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

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

The probability is:

- **Modulated through a temperature parameter T:**
  - for $T \to \infty$ the probability of any move approaches 1
  - for $T \to 0$

- **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 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

```
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 ΔE > 0 then current ← next
      else current ← next only with probability e^(ΔE/T)
```



# Simulated annealing algorithm

- **Simulated annealing algorithm**
  - developed originally for modeling physical processes (Metropolis et al, 53)
  - Metal cooling and crystallization.

    Fast cooling → many faults → higher energy
  - Energy minimization (as opposed of maximization in the previous slides)
- **Properties of the simulated annealing methods**
  - **If temperature T is decreased slowly enough the best configuration (state) is always reached**
- **Applications:** (very large optimization problems)
  - 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 configurations may lead to a configuration with higher value

  (**Not guaranteed !!! )**

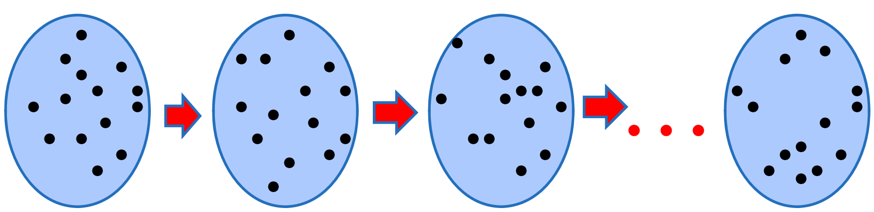
This is the idea behind **genetic algorithms** in which we grow a population of candidate solutions generated from combination of previous configuration candidates



## Genetic algorithms

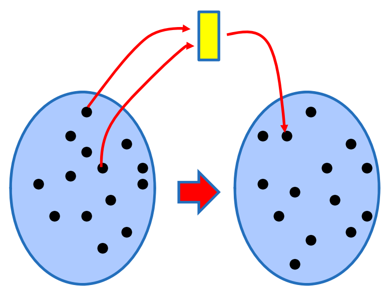
**Algorithm idea:**

- **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**



# Genetic algorithms

- **Selection of configurations to be combined to generate the new population:**
  - **Fitness function = value of the objective function**
  - measures the quality of an individual (a state) in the population



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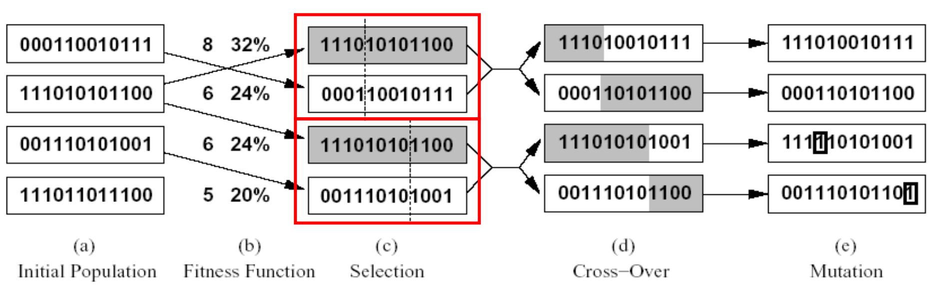
# Reproduction process in GA

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

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