Simulated Annealing

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Iterative Improvement 1

- General method to solve combinatorial optimization problems

Principle:

- Start with initial configuration
- Repeatedly search neighborhood and select a neighbor as candidate
- Evaluate some cost function (or fitness function) and accept candidate if "better"; if not, select another neighbor
- Stop if quality is sufficiently high, if no improvement can be found or after some fixed time

Iterative Improvement 2

Needed are:

- A method to generate initial configuration
- A transition or generation function to find a neighbor as next candidate
- A cost function
- An Evaluation Criterion
- A Stop Criterion

Iterative Improvement 3

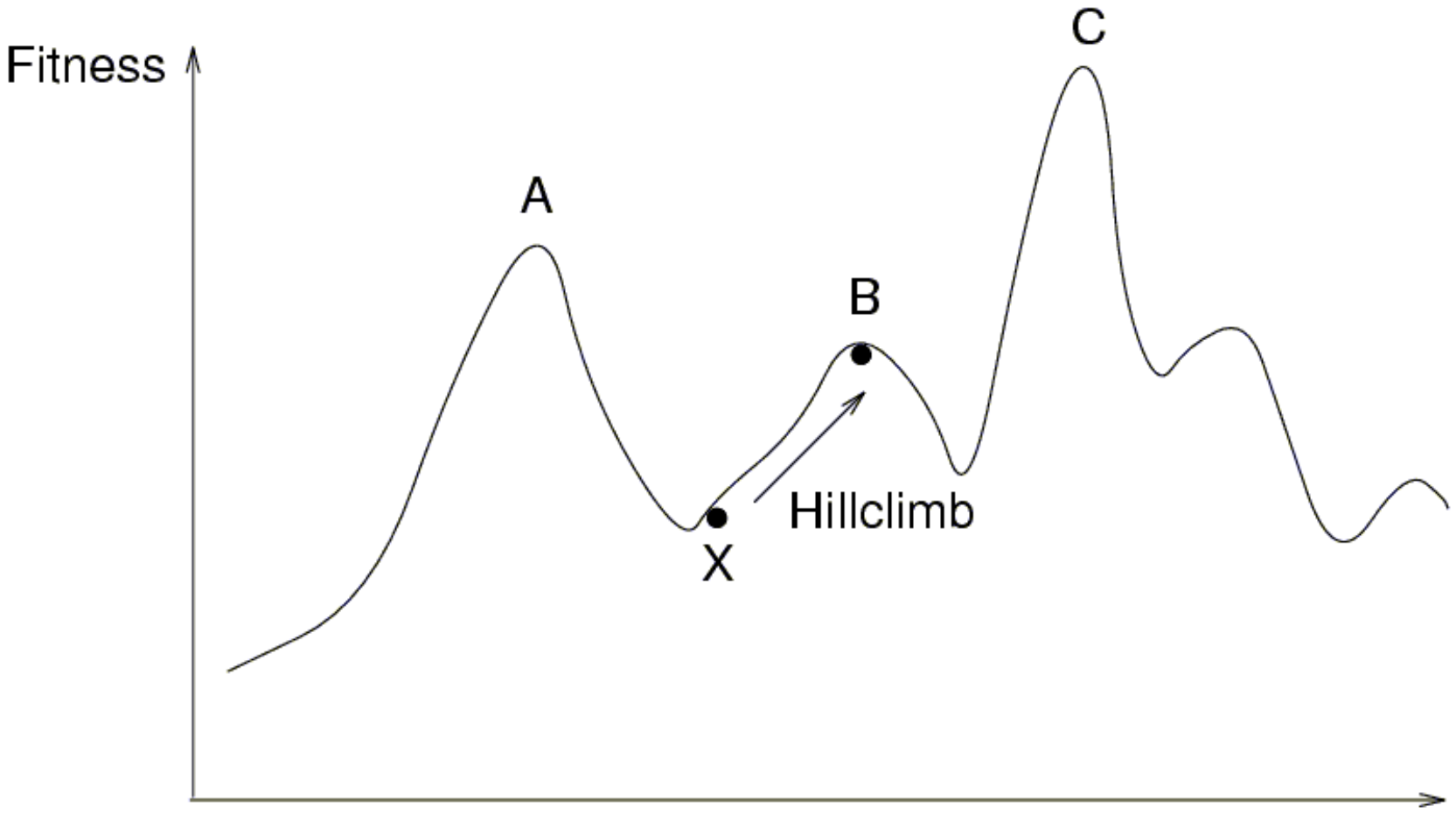
Simple Iterative Improvement or Hill Climbing:

- Candidate is always and only accepted if cost is lower (or fitness is higher) than current configuration
- Stop when no neighbor with lower cost (higher fitness) can be found

Disadvantages:

- Local optimum as best result
- Local optimum depends on initial configuration
- Generally no upper bound on iteration length

Hill climbing



How to cope with disadvantages

- Repeat algorithm many times with different initial configurations
- Use information gathered in previous runs
- Use a more complex Generation Function to jump out of local optimum
- Use a more complex Evaluation Criterion that accepts sometimes (randomly) also solutions away from the (local) optimum

Simulated Annealing

Use a more complex Evaluation Function:

- Do sometimes accept candidates with higher cost to escape from local optimum
- Adapt the parameters of this Evaluation Function during execution
- Based upon the analogy with the simulation of the annealing of solids

Other Names

- Monte Carlo Annealing
- Statistical Cooling
- Probabilistic Hill Climbing
- Stochastic Relaxation
- Probabilistic Exchange Algorithm

Analogy

- Slowly cool down a heated solid, so that all particles arrange in the ground energy state
- At each temperature wait until the solid reaches its thermal equilibrium
- Probability of being in a state with energy E :

$$Pr \{ \mathbf{E} = E \} = 1/Z(T) \, . \, exp \, (-E / k_B.T)$$

E	Energy
T	Temperature
k_B	Boltzmann constant
$Z(T)$	Normalization factor (temperature dependant)

Simulation of cooling (Metropolis 1953)

- At a fixed temperature T :
- Perturb (randomly) the current state to a new state

$\forall$ ΔE is the difference in energy between current and new state

- If $\Delta E < 0$ (new state is lower), accept new state as current state
- If $\Delta E \geq 0$, accept new state with probability

  $Pr\ (accepted) = exp\ (- \Delta E / k_B.T)$
- Eventually the systems evolves into thermal equilibrium at temperature T ; then the formula mentioned before holds
- When equilibrium is reached, temperature T can be lowered and the process can be repeated

Simulated Annealing

- Same algorithm can be used for combinatorial optimization problems:
- Energy *E* corresponds to the Cost function *C*
- Temperature *T* corresponds to control parameter *c*

$$Pr\{\text{configuration} = i\} = 1/Q(c) \cdot \exp(-C(i)/c)$$

C	Cost
c	Control parameter
Q(c)	Normalization factor (not important)

Homogeneous Algorithm

```
initialize;
REPEAT
  REPEAT
    perturb ( config.i → config.j, ΔC_ij);
    IF ΔC_ij < 0 THEN accept
    ELSE IF exp(-ΔC_ij/c) > random[0,1) THEN accept;
    IF accept THEN update(config.j);
  UNTIL equilibrium is approached sufficient closely;
  c := next_lower(c);
UNTIL system is frozen or stop criterion is reached
```

Inhomogeneous Algorithm

- Previous algorithm is the homogeneous variant:

  c is kept constant in the inner loop and is only decreased in the outer loop

- Alternative is the inhomogeneous variant:

  There is only one loop; *c* is decreased each time in the loop, but only very slightly

Parameters

- Choose the start value of *c* so that in the beginning nearly all perturbations are accepted (exploration), but not too big to avoid long run times
- The function *next_lower* in the homogeneous variant is generally a simple function to decrease *c*, e.g. a fixed part (80%) of current *c*
- At the end *c* is so small that only a very small number of the perturbations is accepted (exploitation)

- If possible, always try to remember explicitly the best solution found so far; the algorithm itself can leave its best solution and not find it again

Markov Chains 1

Markov Chain:

Sequence of trials where the outcome of each trial depends only on the outcome of the previous one

- Markov Chain is a set of conditional probabilities:

  $P_{ij}(k-1,k)$

  Probability that the outcome of the *k*-th trial is *j*, when trial *k-1* is *i*

- Markov Chain is homogeneous when the probabilities do not depend on k

Markov Chains 2

- When c is kept constant (homogeneous variant), the probabilities do not depend on k and for each c there is one homogeneous Markov Chain

- When c is not constant (inhomogeneous variant), the probabilities do depend on k and there is one inhomogeneous Markov Chain

Performance

- SA is a general solution method that is easily applicable to a large number of problems
- "Tuning" of the parameters (initial *c*, decrement of *c*, stop criterion) is relatively easy
- Generally the quality of the results of SA is good, although it can take a lot of time
- Results are generally not reproducible: another run can give a different result
- SA can leave an optimal solution and not find it again (so try to remember the best solution found so far)
- Proven to find the optimum under certain conditions; one of these conditions is that you must run forever