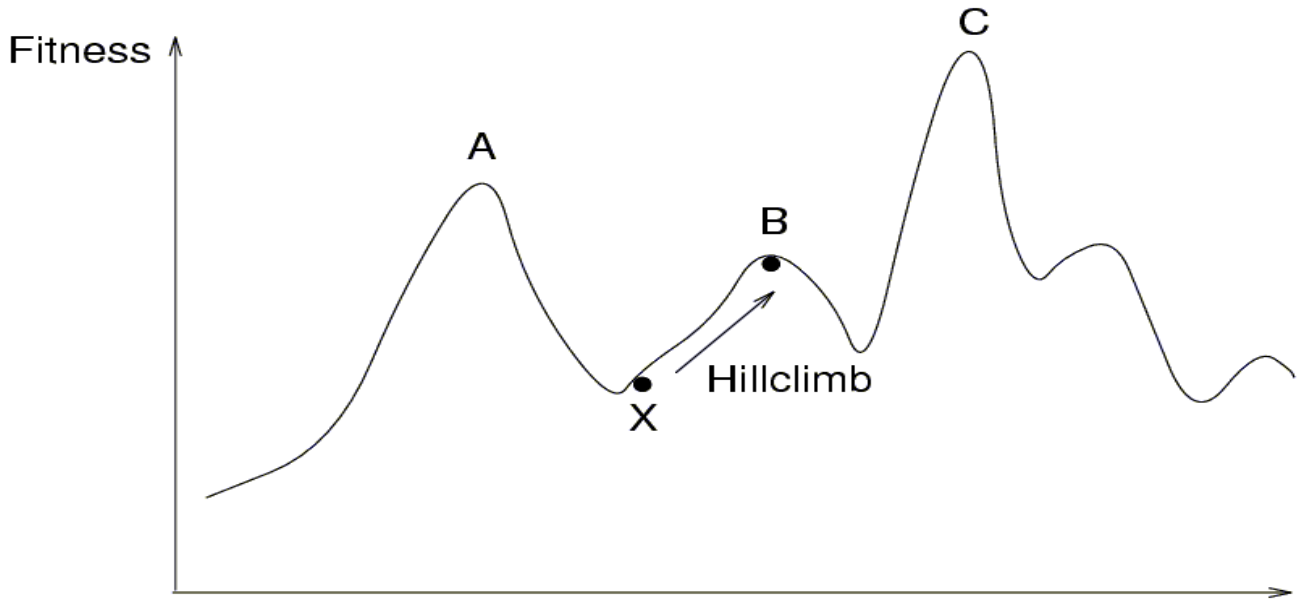
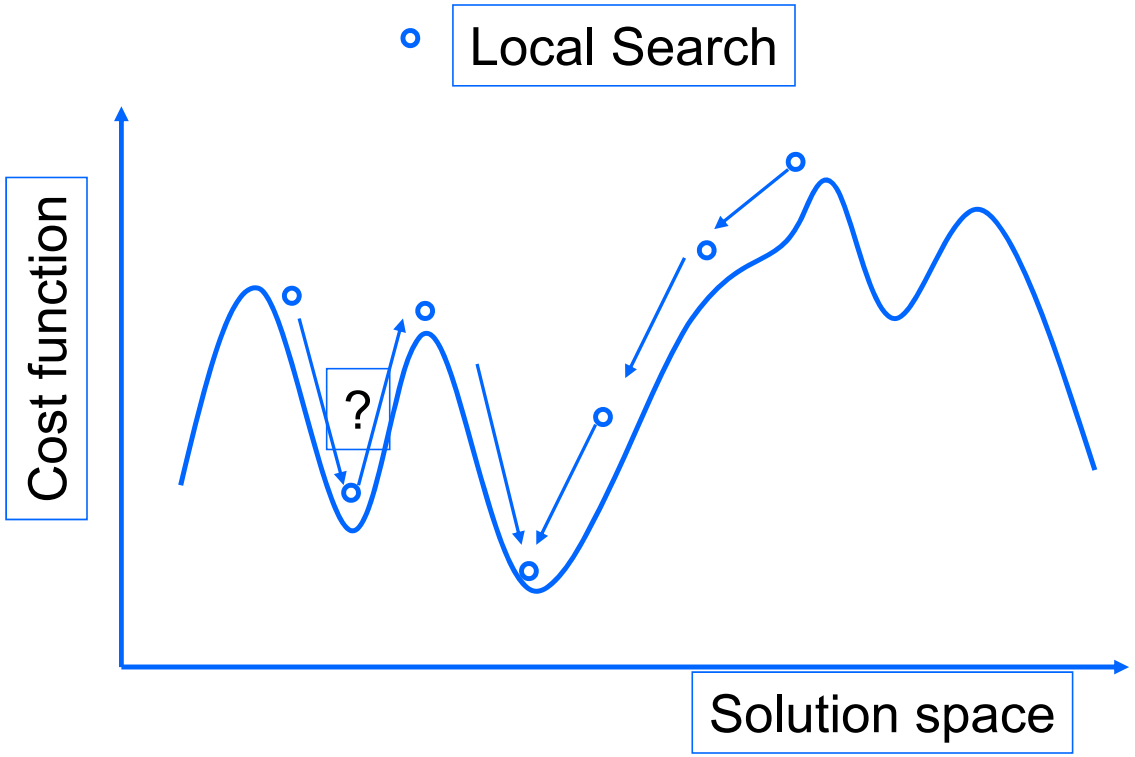
Simulated Annealing

Hill climbing



Simulated Annealing



Annealing

- Annealing is a thermal process for obtaining low energy states of a solid in a heat bath.

- The process contains two steps:
  - Increase the temperature of the heat bath to a maximum value at which the solid melts.
  - Decrease carefully the temperature of the heat bath until the particles arrange themselves in the ground state of the solid. Ground state is a minimum energy state of the solid.

- The ground state of the solid is obtained only if the maximum temperature is high enough and the cooling is done slowly.


1cm

Simulated Annealing

- To apply simulated annealing with optimization purposes we require the following:
  - A successor function that returns a “close” neighboring solution given the actual one. This will work as the “disturbance” for the particles of the system.
  - A target function to optimize that depends on the current state of the system. This function will work as the energy of the system.

- The search is started with a randomized state. In a polling loop we will move to neighboring states always accepting the moves that decrease the energy while only accepting bad moves accordingly to a probability distribution dependent on the “temperature” of the system.

Simulated Annealing

- Decrease the temperature slowly, accepting less bad moves at each temperature level until at very low temperatures the algorithm becomes a greedy hill-climbing algorithm.
  - The distribution used to decide if we accept a bad movement is know as Boltzman distribution.

$$P(\gamma) = \frac{e^{-E_\gamma/T}}{Z(T)},$$

$$Z(T) = \sum_{\gamma'} e^{-E_{\gamma'}/T},$$

  - This distribution is very well known is in solid physics and plays a central role in simulated annealing. Where γ is the current configuration of the system, E_γ is the energy related with it, and Z is a normalization constant.

Annealing Process

- Annealing Process
  - **Raising the temperature up** to a very high level (melting temperature, for example), the atoms have a higher energy state and ***a high possibility to re-arrange the crystalline*** structure.

  - **Cooling down slowly**, the atoms have a *lower and lower energy state* and a smaller and smaller possibility to re-arrange the crystalline structure.

Statistical Mechanics

Combinatorial Optimization

State {r:} (configuration -- a set of atomic position)

weight $e^{-E(\{r:\})/K_B T}$ **-- Boltzmann distribution**

E({r:]): energy of configuration

K_B: Boltzmann constant

T: temperature

Low temperature limit ??

Analogy

Physical System		Optimization Problem
State (configuration)	→	Solution
Energy	→	Cost function
Ground State	→	Optimal solution
Rapid Quenching	→	Iteration improvement
Careful Annealing	→	Simulated annealing

Simulated Annealing

- ***Analogy***
  - Metal ←→ Problem
  - Energy State ←→ Cost Function
  - Temperature ←→ Control Parameter
  - A completely ordered crystalline structure ←→ the optimal solution for the problem

Global optimal solution can be achieved as long as the cooling process is slow enough.

Other issues related to simulated annealing

1. **Global optimal** solution is possible, but near optimal is practical

2. Parameter Tuning
    1. Aarts, E. and Korst, J. (1989). *Simulated Annealing and Boltzmann Machines*. John Wiley & Sons.

3. Not easy for parallel implementation, but was implemented.

4. **Random generator quality is important**

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 :

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

E	Energy
T	Temperature
k_B	Boltzmann constant
$\mathbf{Z(T)}$	Normalization factor (temperature dependant)

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)

Components of Simulated Annealing

- Definition of solution
- Search mechanism, i.e. the definition of a neighborhood
- Cost-function

Control Parameters

1. How to define equilibrium?
2. How to calculate new temperature for next step?

1. Definition of equilibrium
   1. Definition is reached when we cannot yield any significant improvement after certain number of loops
   2. A constant number of loops is assumed to reach the equilibrium

2. Annealing **schedule** (i.e. How to reduce the temperature)
   1. A constant value is subtracted to get new temperature, $T' = T - T_d$
   2. A constant scale factor is used to get new temperature, $T' = T * R_d$
      - A scale factor usually can achieve better performance

Control Parameters: Temperature

- Temperature determination:
  - Artificial, without physical significant
  - **Initial** temperature
    1. Selected so high that leads to 80-90% acceptance rate
  - **Final** temperature
    1. Final temperature is a constant value, i.e., based on the total number of solutions searched. No improvement during the entire Metropolis loop
    2. Final temperature when acceptance rate is falling below a given (small) value

- *Problem specific* and may need to be tuned

Simulated Annealing: the code

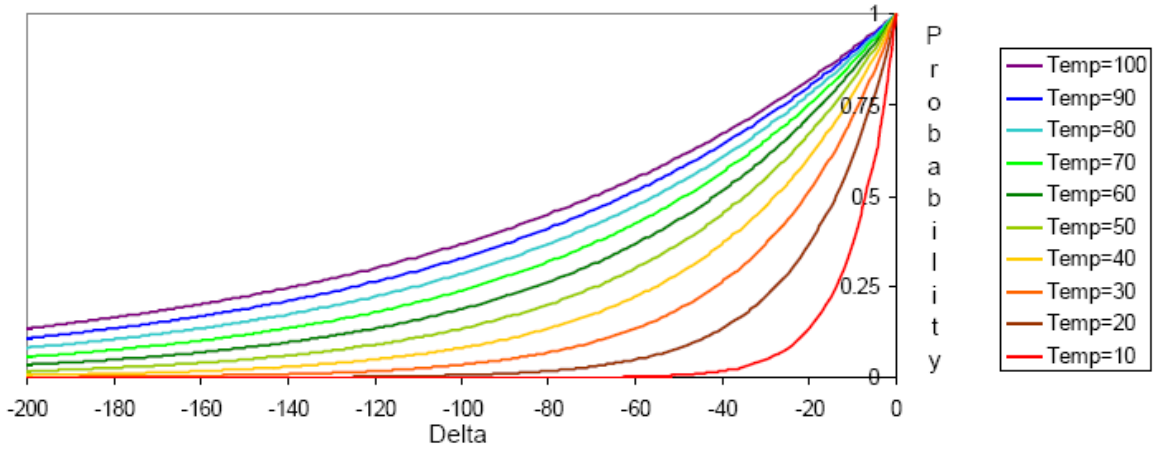
```
1. Create random initial solution γ
2. E_old=cost(γ);
3. for(temp=temp_max; temp>=temp_min;temp=next_temp(temp) ) {
4.    for(i=0;i<i_max; i++ ) {
5.          succesor_func(γ); //this is a randomized function
6.          E_new=cost(γ);
7.          delta=E_new-E_old;
8.          if(delta>0)
9.                if(random() >= exp(-delta/K*temp);
10.                     undo_func(γ); //rejected bad move
11.               else
12.                    E_old=E_new  //accepted bad move
13.         else
14.               E_old=E_new; //always accept good moves
       }
    }
```

Simulated Annealing

- Acceptance criterion and cooling schedule

if (delta>=0) accept

else if ($random < e^{delta/Temp}$) accept, else reject /* 0<=random<=1 */



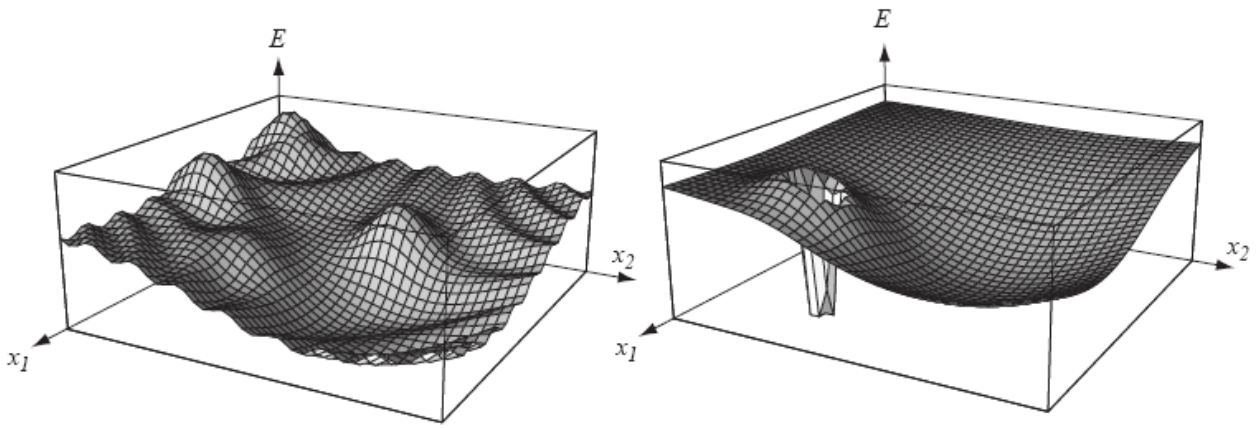
Initially temperature is very high (most bad moves accepted)

Temp slowly goes to 0, with multiple moves attempted at each temperature

Final runs with temp=0 (always reject bad moves) greedily “quench” the system

Practical Issues with simulated annealing

- Cost function must be carefully developed, it has to be “fractal and smooth”.
- The energy function of the left would work with SA while the one of the right would fail.



Practical Issues with simulated annealing

- The cost function should be fast it is going to be called “millions” of times.
- The best is if we just have to calculate the deltas produced by the modification instead of traversing through all the state.
- This is dependent on the application.

Practical Issues with simulated annealing

- In asymptotic convergence simulated annealing converges to globally optimal solutions.
- In practice, the convergence of the algorithm depends of the cooling schedule.
- There are some suggestion about the cooling schedule but it stills requires a lot of testing and it usually depends on the application.

Practical Issues with simulated annealing

- Start at a temperature where 50% of bad moves are accepted.
- Each cooling step reduces the temperature by 10%
- The number of iterations at each temperature should attempt to move between 1-10 times each “element” of the state.
- The final temperature should not accept bad moves; this step is known as the quenching step.

Applications

- Basic Problems
  - Traveling salesman
  - Graph partitioning
  - Matching problems
  - Graph coloring
  - Scheduling

- Engineering
  - VLSI design
    - Placement
    - Routing
    - Array logic minimization
    - Layout
  - Facilities layout
  - Image processing
  - Code design in information theory

Example of Simulated Annealing

- Traveling Salesman Problem (TSP)
  - Given 6 cities and the traveling cost between any two cities
  - A salesman need to start from city 1 and travel all other cities then back to city 1
  - Minimize the total traveling cost

Example: SA for traveling salesman

- Solution representation
  - An integer list, i.e., (1,4,2,3,6,5)
- Search mechanism
  - Swap any two integers (except for the first one)
    - (1,4,2,3,6,5) → (1,4,3,2,6,5)
- Cost function

Example: SA for traveling salesman

- Temperature
  1. Initial temperature determination
     1. Initial temperature is set at such value that there is around 80% acceptation rate for "bad move"
     2. Determine acceptable value for ($C_{new} - C_{old}$)
  2. Final temperature determination
     - Stop criteria
     - Solution space coverage rate

- Annealing **schedule** (i.e. How to reduce the temperature)
  - A constant value is subtracted to get new temperature, $T' = T - T_d$
    - For instance new value is 90% of previous value.
      - Depending on solution space coverage rate

Simulated Annealing

- The process of annealing can be simulated with the Metropolis algorithm, which is based on Monte Carlo techniques.
- We can apply this algorithm to generate a solution to combinatorial optimization problems assuming an analogy between them and physical many-particle systems with the following equivalences:
  - Solutions in the problem are equivalent to states in a physical system.
  - The cost of a solution is equivalent to the “energy” of a state.

Simulated Annealing Algorithm

Initialize:

- initial solution **x** ,
- highest temperature $\mathbf{T_h}$,
- and coolest temperature $\mathbf{T_l}$

$\mathbf{T = T_h}$

When the temperature is higher than $\mathbf{T_l}$

  While not in equilibrium

    Search for the new solution **X'**

    Accept or reject **X'** according to Metropolis Criterion

  End

  Decrease the temperature **T**

End