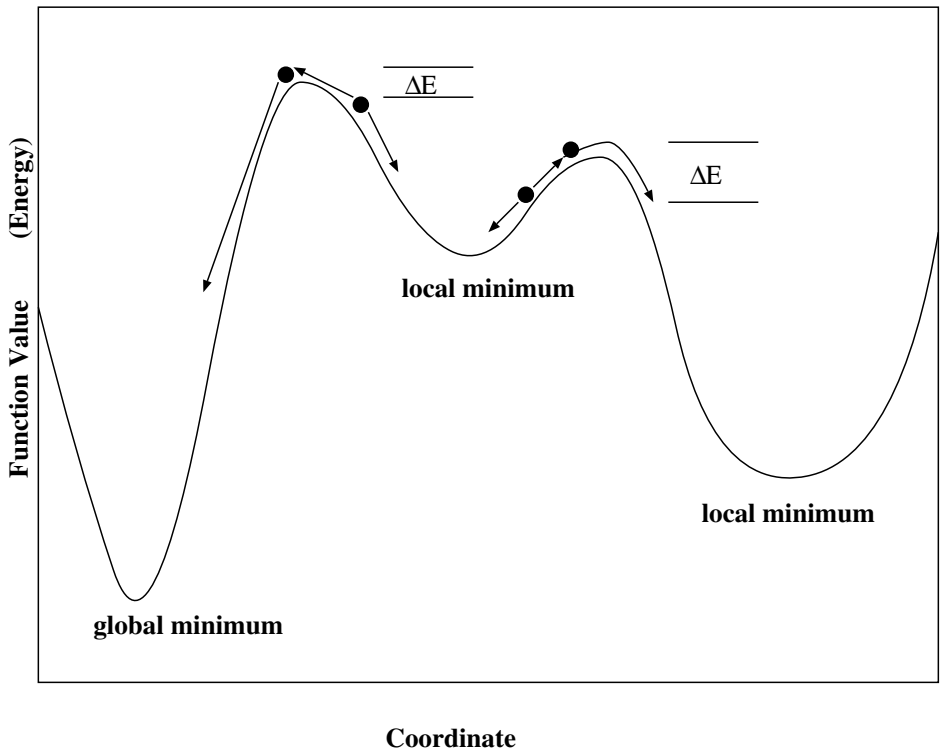
Monte Carlo Methods: Global Minimum



Anologies

State	Feasible Solution
Energy	Cost
Ground State	Optimal Solution
Rapid Quenching	Local Search
Careful Annealing	Simulated Annealing

Boltzmann Annealing

Three Functional Relationships
$x = \{ x_1, x_2, ..., x_D \}$

$g(a)$
Probability Density of state-space

$h(x)$
Probability Density for Acceptance

$T(k)$
Schedule of adjusting T temperature
in terms of k steps

Acceptance

The key to the methods

Though prefers going downhill

Allow Climbing uphill

Based on Boltzmann's Statistics
Statistical Mechanic Energy Partitions

The chances of obtaining a new state with energy
E_{k+1} given E_k

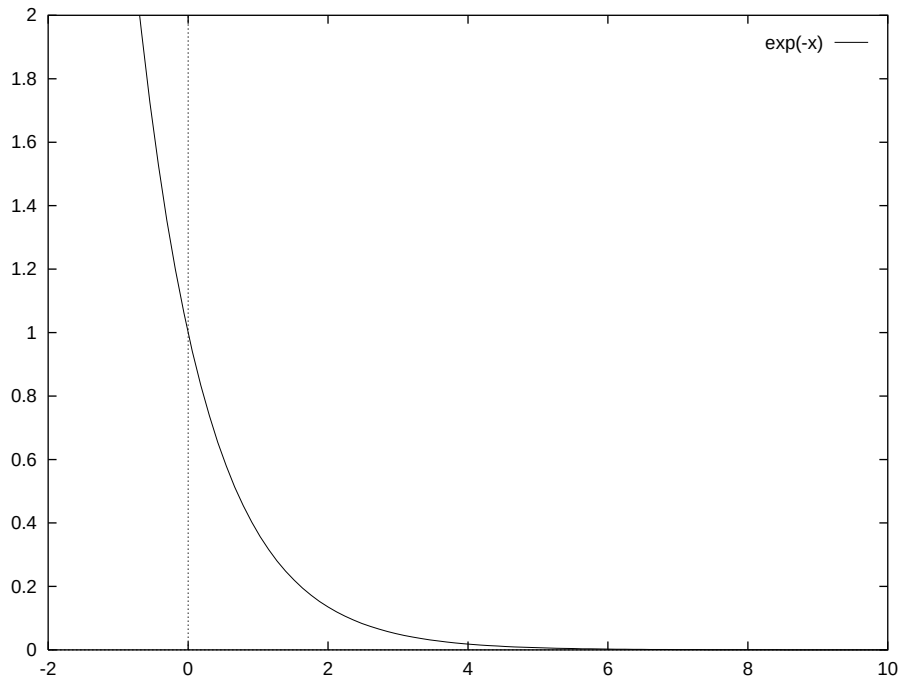
$$e^{\frac{1}{1+-e\nabla E}T}$$

approximately equal to

$$e_{\frac{-\nabla E}{T}}$$
$$\nabla E = E_{k+1} - E_k$$

Finite Chance that energy will be greater than zero

Probability



Use in Monte Carlo Method

Define:
$h(\nabla x)$

For ∇x less than zero
(i.e. a decrease in value)
Probability of acceptance is one
(i.e. always accept the result)

For ∇x greater than zero
(i.e. an increase in value)
Probability is less than one: $e^{\frac{-\nabla x}{T}}$
(i.e. sometimes accept the result)

Use in Monte Carlo Method

T

A constant which reflects to what degrees uphill climbs should be accepted

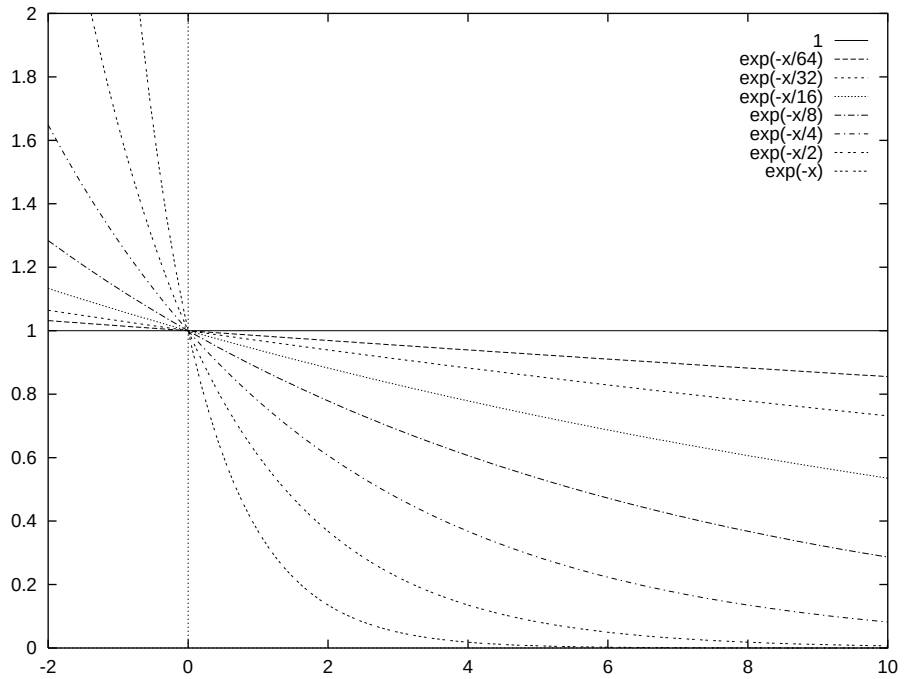
How to accept or reject result?

Compare with a random number between zero and one: $random_i$

if $h(x) \geq random_i$ **Accept** new point

if $h(x) < random_i$ **Reject** new point

The role of T


2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
-2
0
2
4
6
8
10
1
exp(-x/64)
exp(-x/32)
exp(-x/16)
exp(-x/8)
exp(-x/4)
exp(-x/2)
exp(-x)

The Role of T

For Large *Temperatures*

More Uphill Solutions will be accepted

Allows wandering through the state space

Can jump out of local minimum trap

For Small *Temperatures*

Most likely only to accept downhill solutions

Stays within minimum

Annealing Schedule

Metropolis Algorithm

Provide a scheduling of Temperatures
through the set of interations

Start at a high temperature
to allow wandering through the whole space of solutions

Slowly lower the temperature
to damp the acceptance of uphill climbs

Traveling Saleman Problem

One of the Classic Successes of Simulated Annealing

Problem

The salesman visits N cities with given positions (x_i, y_i) and return to the city of origin.

Each City is to visited only once

The route is to be as short as possible

NP-Complete
Complexity Increases Rapidly as N increases

There are many local minima