SIMULATED ANNEALING

An Heuristic for Combinatorial Optimization Problems

Annealing

- A metal is strongest in the purest crystalline state
- Restated: A metal is strongest in the lowest energy state

Annealing

- Cooling molecules will sometimes find an adjacent lower energy state, when, in fact, a state even lower may not be adjacent.
- Cooling to the adjacent lower state may lead to an imperfect crystalline state ultimately (not the lowest energy state possible)

Annealing

- The process of annealing involves heating the metal to a very high temperature, then letting it cool SLOWLY.
- By slow cooling, molecules can jump about in the structure, leaping over adjacent higher energy boundaries, to find ultimately lower energy states; in fact, the molecules with higher energy can travel the landscape before cooling.

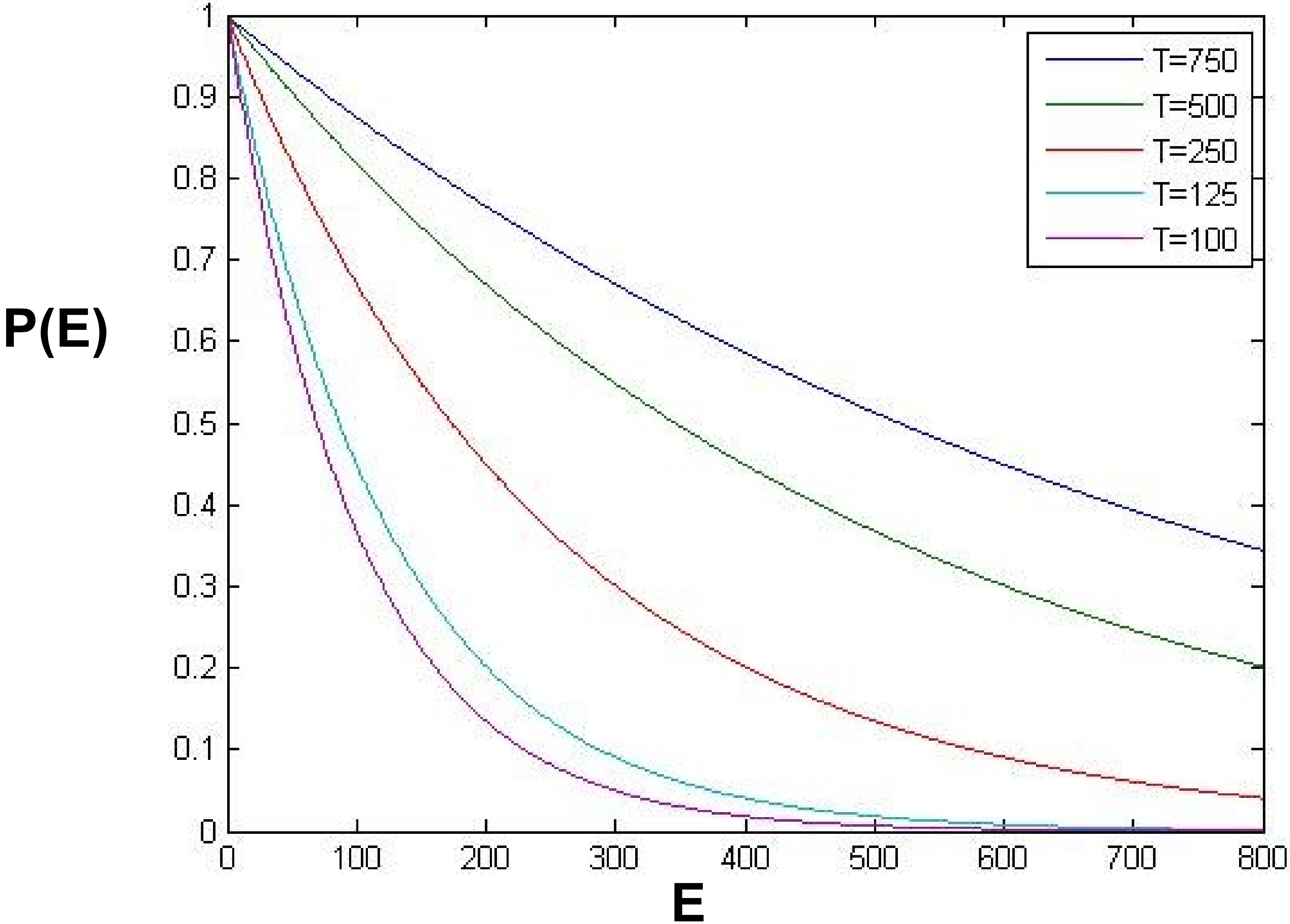
Annealing

The Boltzmann density gives the probability of being in some energy state *p(E),* given that energy state *E,* and the temperature *T*

$$p(E) = e^{\frac{-TE}{k}}$$

Where *k* is Boltzmann's constant

Effect of temperature on probability in the Boltzmann relationship



KEY CONCEPT

Annealing works because molecules can jump out of energy local minima, over energy barriers, towards a global minimum. The jumping happens with a probability that is related both to the current energy state and the current temperature

Simulated Annealing Models Annealing

The SA algorithm has four elements

- Definition of a cost function
- Definition and selection of configurations
- Definition of an annealing schedule
- Definition of a scheme for making energetically unfavorable steps

Simulated Annealing

The algorithm:

- At each temperature, for sufficient iterations:
  - Select a configuration (choose a neighborhood)
  - Compute the cost function
    - If the cost is lowered, keep the configuration
    - If it is higher, keep it only with a certain (Boltzmann) probability (the Metropolis step)
- Reduce the temperature

Instead of only accepting a neighbor s_j of the current solution s_i as the new starting point for further search steps when

$$f(s_j) \leq f(s_i)$$

SA also accepts the new solution s_j when its objective function value is actually ***worse*** than the old one's, but in this case only with the so-called Metropolis probability

$$p_{accepting} \leq e^{-\frac{f(s_j)-f(s_i)}{T}}$$

which is a decreasing function of the difference in objective function values and an increasing function of a virtual control variable T, called temperature

Key factors in Algorithm Design

- Iterations at a given temperature
- Cooling Schedule
- Choice of configurations
  - Reversals, Swaps with distance data
  - How to choose among configuration strategies?

TSP Demo

Look in Tools,Tables and Templates on our website for a Simulated Annealing demo of the TSP

http://bioinformatics.uchc.edu/Bioinformatics_tools/BioInfo_SimulatedAnnealing.aspx

TSP: 23 Cities Alphabetical

Temp

Iterations at this temp

5000

Total Iterations

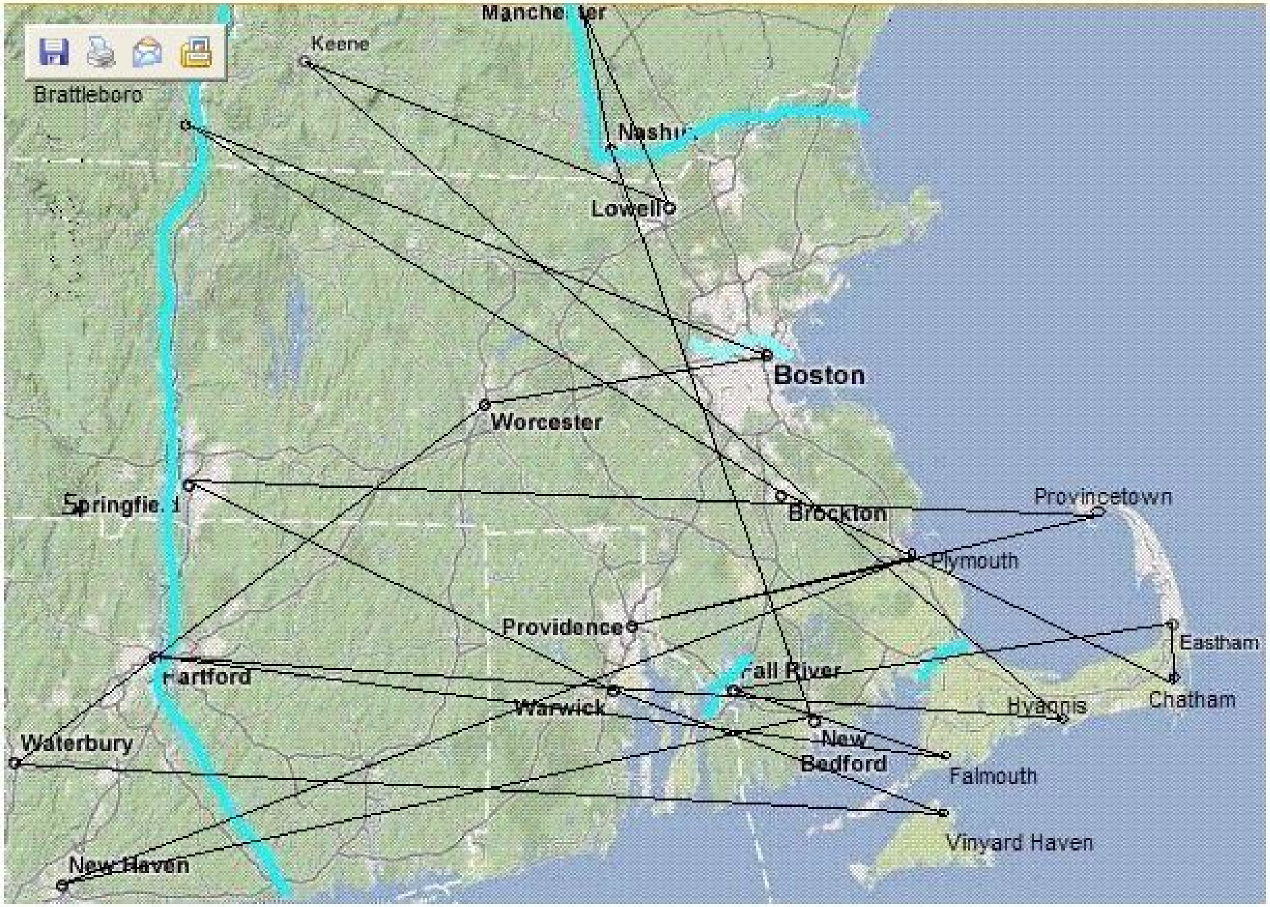
Label

Number of Metropolis Steps

Distance

6050.6

Begin Computation



23 Cities 1000°

Temp
1000.00

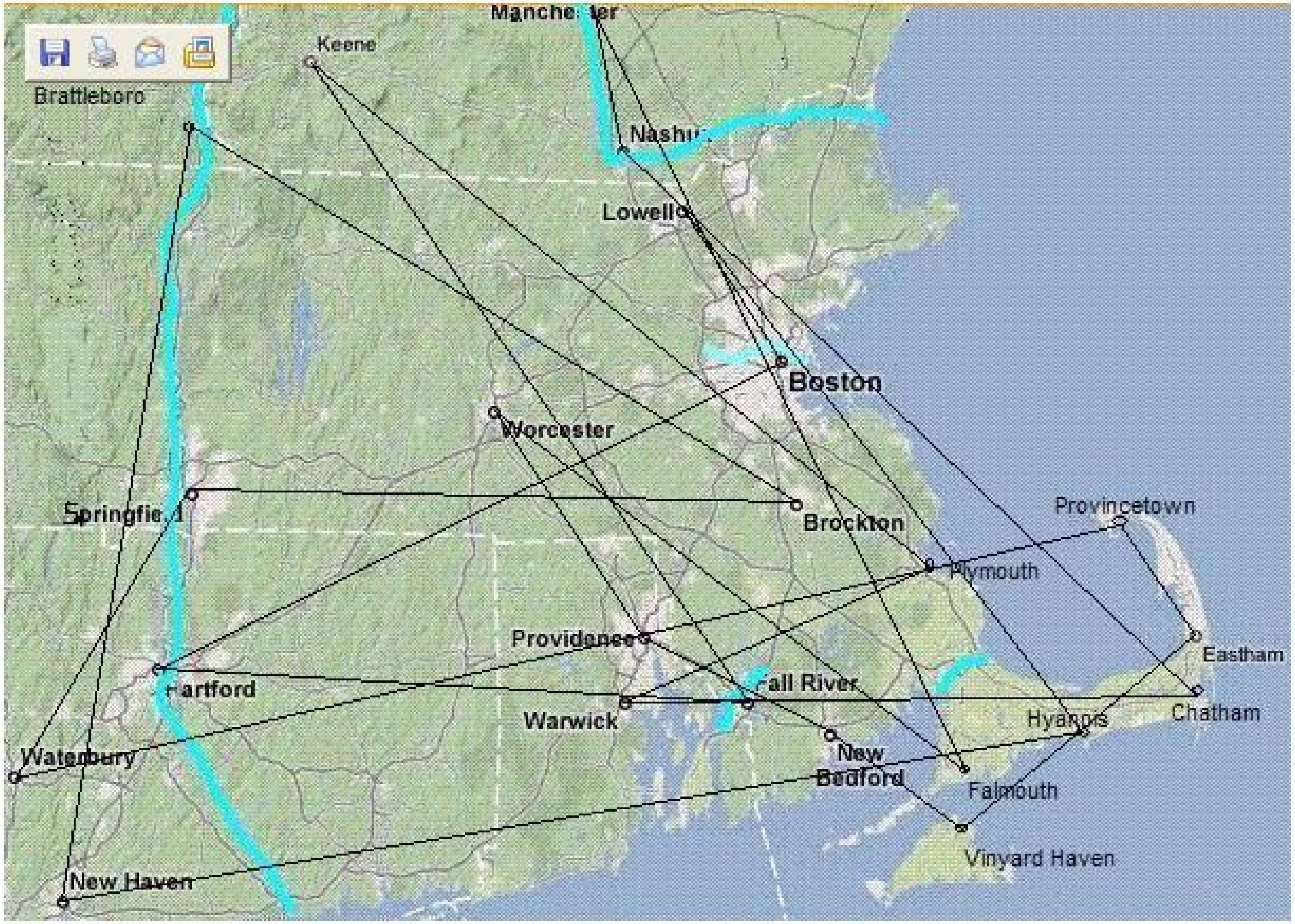
Iterations at this temp
5050

Total Iterations
5050

Number of Metropolis Steps
3692

Distance
6002.3

Decrease Temp



23 Cities 10° 4,329,345 iterations

Temp
9.99

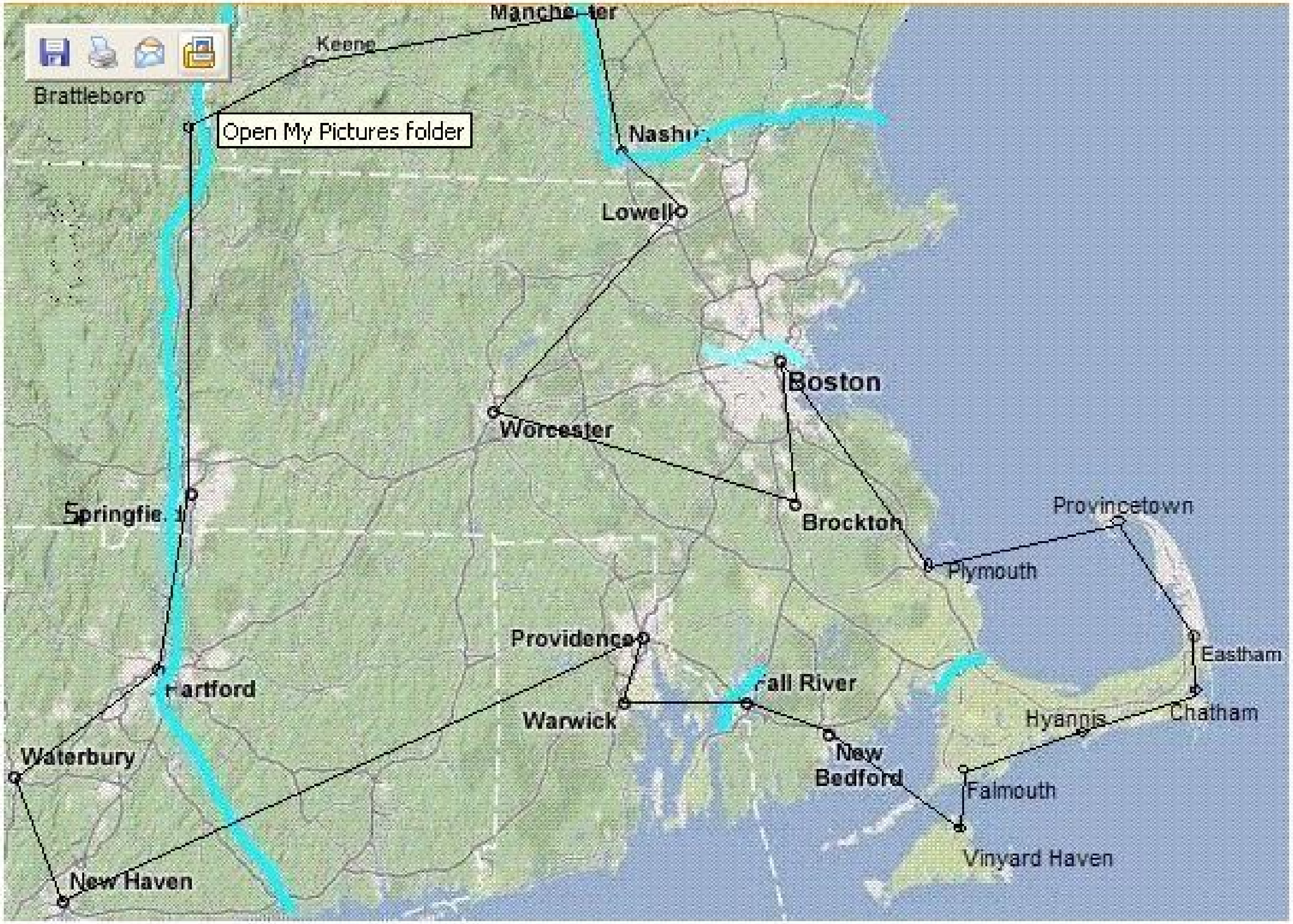
Iterations at this temp
48372

Total Iterations
4392345

Number of Metropolis Steps
24343

Distance
2015.5

Decrease Temp



Solution

- Our Solution
  - 4,329,345 iterations to 10°
- Complete Solution
  - 25,852,016,738,884,976,640,000 iterations

    (~26 sextillion)
  - If a configuration could be resolved in one computer cycle, it would take a 2.2GHz machine 372,619 years to evaluate all unique configurations

SA

- The cost function can allow some sophisticated evaluations, including inclusion of penalties as well as rewards
  - Simple: Water crossing penalty in TSP
  - Complex: Intensity modulated radiotherapy with target/protected structure tradeoffs

Water Crossing Penalty 16.9° 3,278,502 iterations

Temp
16.89

Iterations at this temp
37358

Total Iterations
3278502

Number of Metropolis Steps
18732

Distance
2015.7

Decrease Temp