

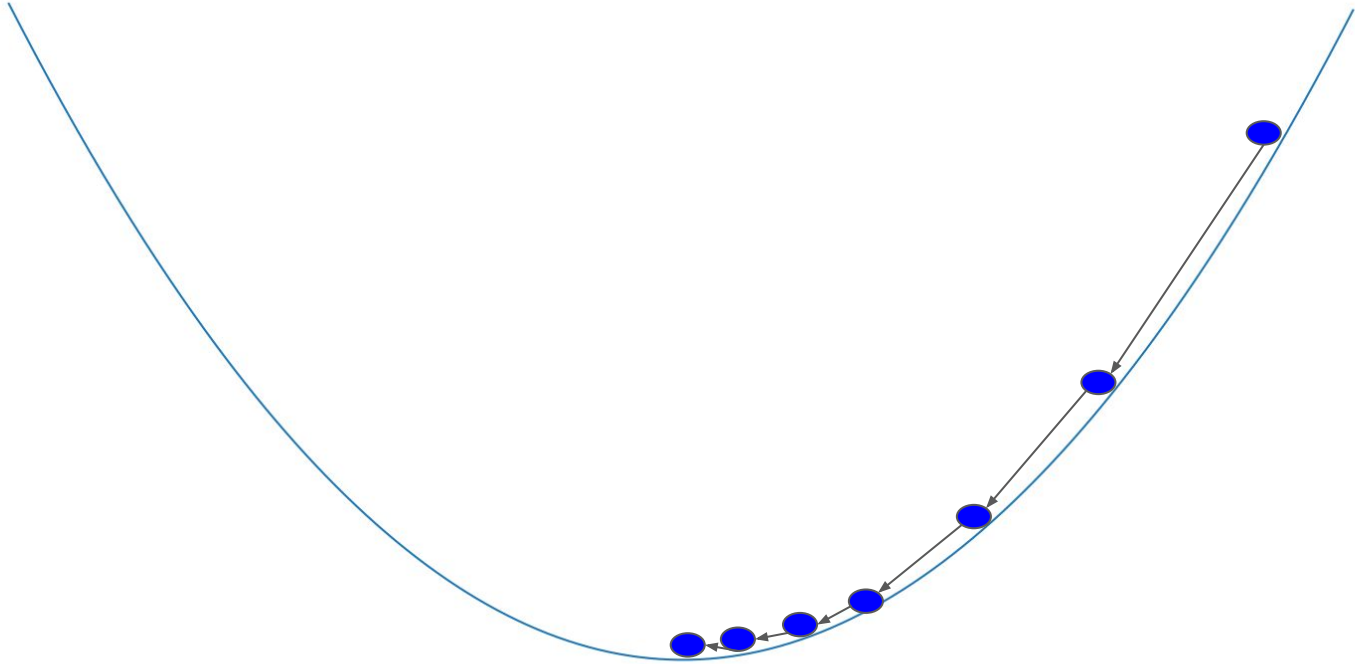
The background image shows the interior of a high-temperature furnace. The walls and ceiling are lined with refractory bricks, glowing with a bright orange and yellow light. The floor is covered with a grid of circular, metallic-looking elements, possibly heating coils or trays, which are also glowing from the heat. The perspective is looking down a long, narrow aisle towards a bright opening at the end of the furnace.

Simulated Annealing

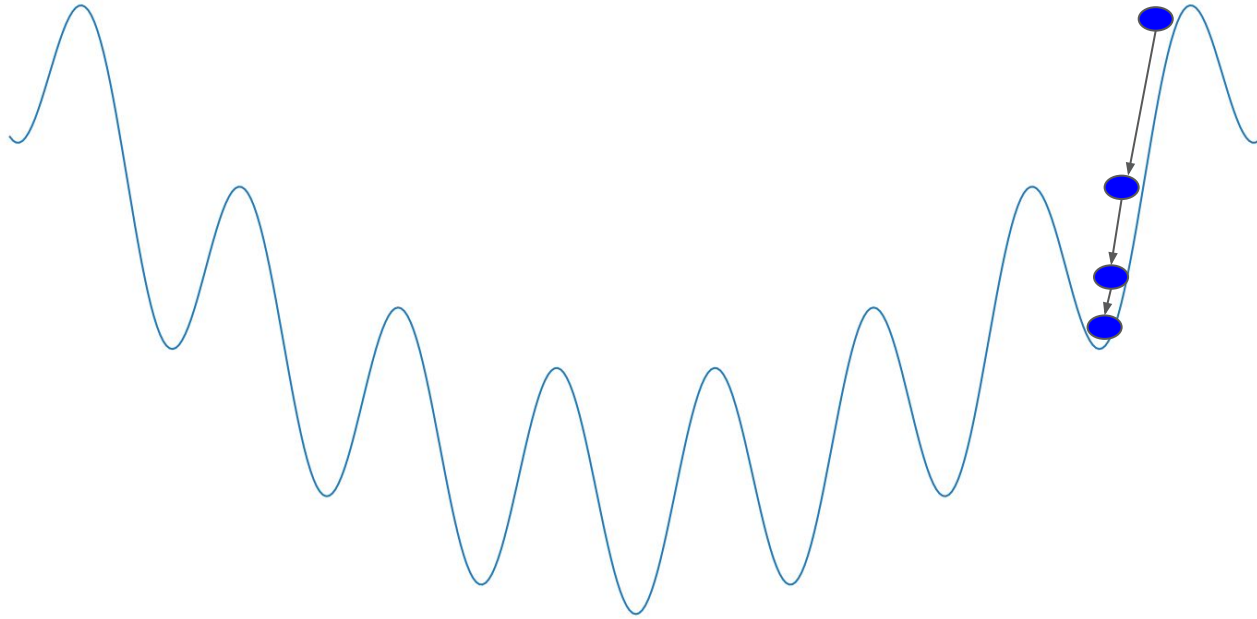
Chad Germany

<http://www.gdfurnace.com/bright-annealing-furnace/high-temperature-continuous-bright-annealing.html>

You have some objective function



An objective function with many minima



Gradient descent fails with many local minima

- It tries to find local optimum (best) solution after every step
- This means that it can get trapped in local minima since it cannot go backwards



Is there another way to optimize functions with many local minima?

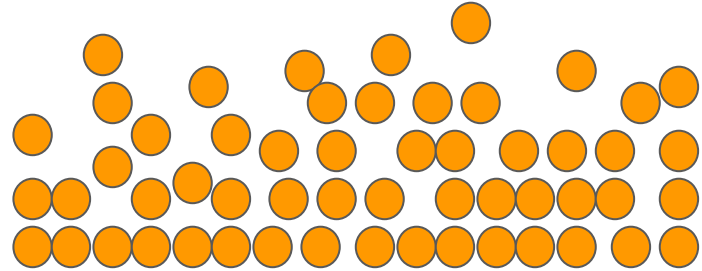
Yes!

One such optimization algorithm is called simulated annealing which is the topic of this talk

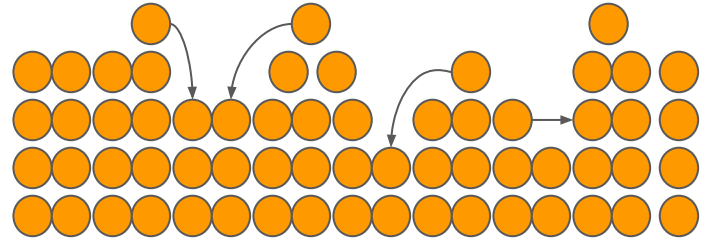
What does it mean to anneal

1. Heating a material above its recrystallization temperature
2. Maintain the temperature for a suitable amount of time
3. Then allow slow cooling

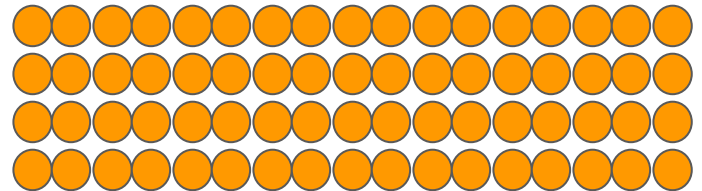
High
Temperature



Slow Cooling



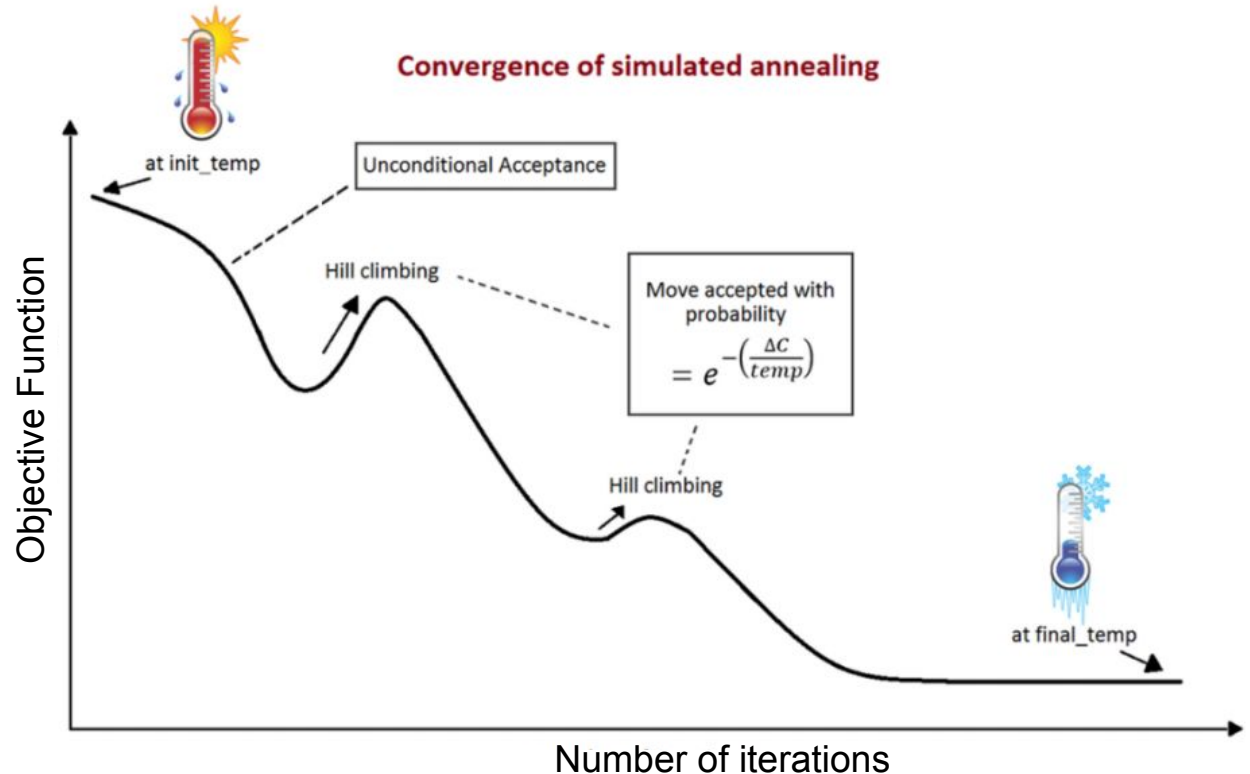
Low
Temperature



reduction of dislocations in the crystal structure of the material being annealed

What the high level view of simulated annealing

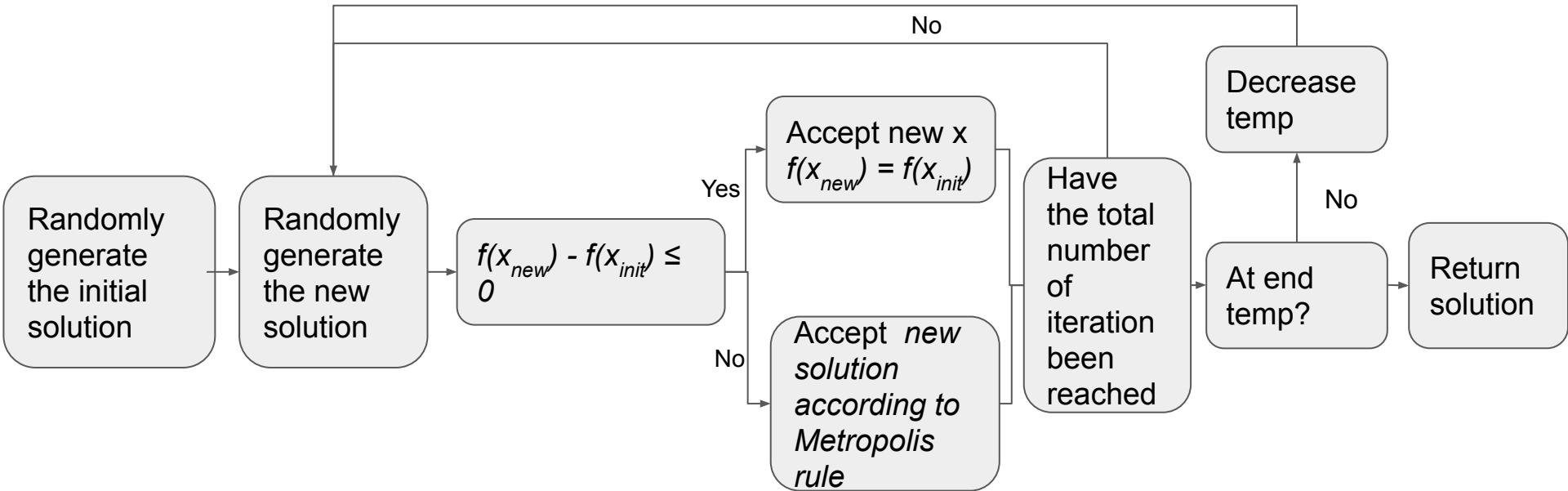
- Optimizing algorithm
- It slowly decreases the probability of accepting worse solutions as the solution space is explored



How do you determine whether simulated annealing is the right tool

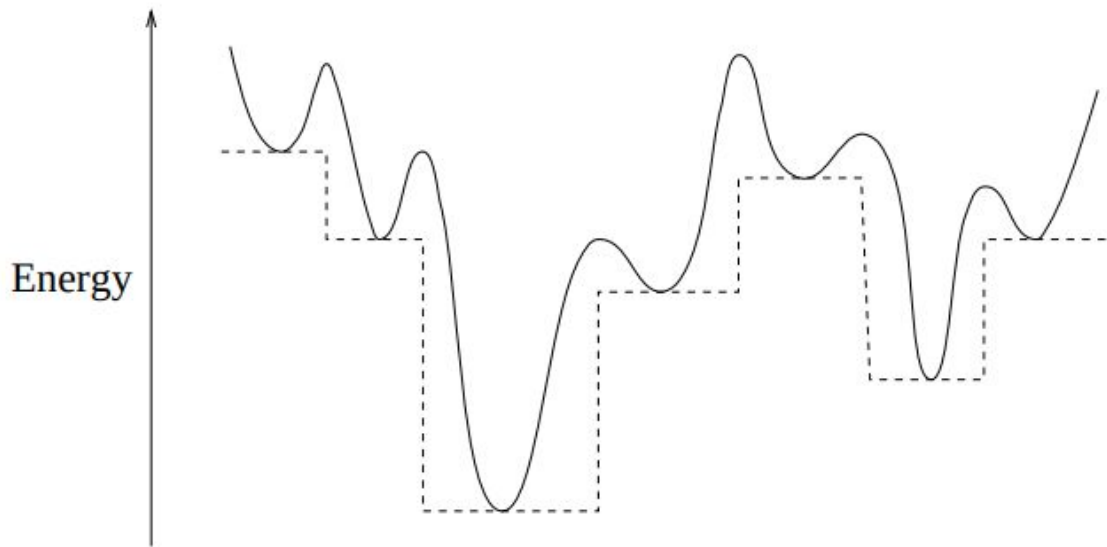
- Determine whether local minima are a problem.
 - Typically this involves greedy searches from a random sample of initial states.
 - If the results are widely different, then it probably pays to do a careful search for the global minimum
- Determine whether the problem warrants exploiting additional structure.
 - This often amounts to the issue of what additional information already exists concerning the problem and algorithms for its solution and how easily this additional information can be implemented in a global optimization algorithm.
- It is in the intermediate regime where simulated annealing finds its niche
 - complex problems whose structure does not warrant further study or that are so hard that analysis is likely to be very slow.
 - It's a good general global optimization algorithm

Algorithm for finding global minimum



How well does this work compared to scipy's basin-hopping

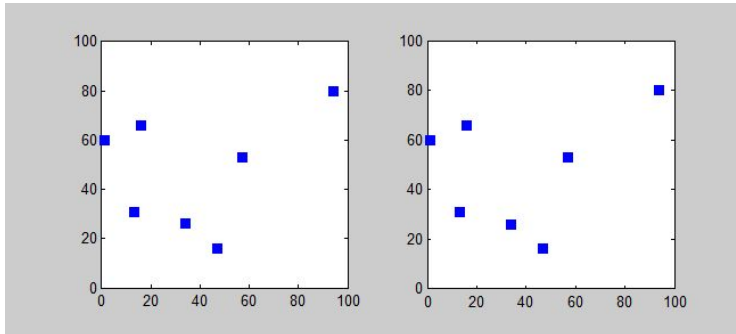
basin-hopping



Travelling salesman problem

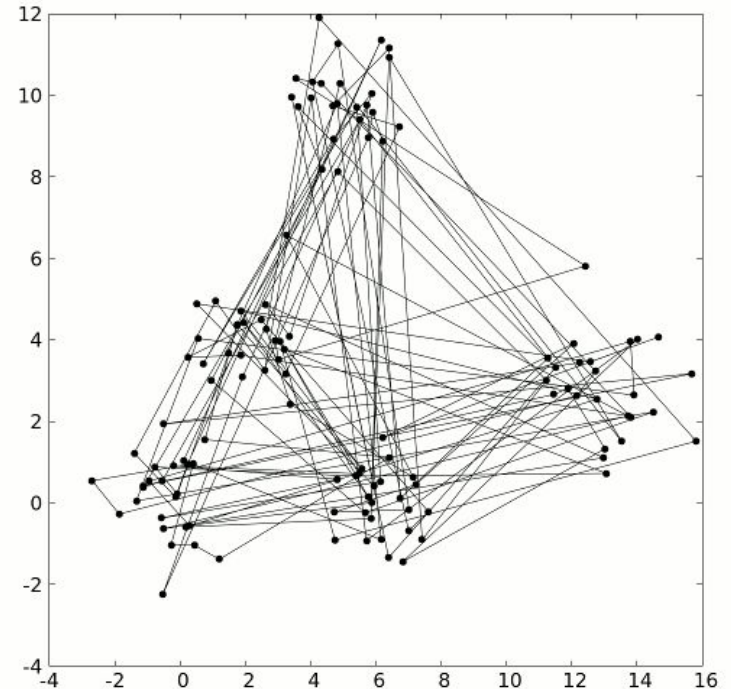
- "Given a list of cities and the distances between each pair of cities, what is the shortest possible route that visits each city and returns to the origin city?"
- It is an NP-Hard problem

Brute force



Simulated Annealing

E= 852 T=125



References

1. Whales and Doye, J. Phys. Chem. A 101, 5111-5116 (1997)
2. https://en.wikipedia.org/wiki/Travelling_salesman_problem
3. <https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.basinhopping.html>
4. Peter Salamon, Paolo Sibani, and Richard Frost, Facts, Conjectures and Improvements for Simulated Annealing

Basin Hopping (extra slide)

Basin-hopping is a stochastic algorithm which attempts to find the global minimum of a smooth scalar function of one or more variables [1] [2] [3] [4]. The algorithm in its current form was described by David Wales and Jonathan Doye [2] <http://www-wales.ch.cam.ac.uk/>.

The algorithm is iterative with each cycle composed of the following features

1. random perturbation of the coordinates
2. local minimization
3. accept or reject the new coordinates based on the minimized function value

The acceptance test used here is the Metropolis criterion of standard Monte Carlo algorithms, although there are many other possibilities [3].

This global minimization method has been shown to be extremely efficient for a wide variety of problems in physics and chemistry. It is particularly useful when the function has many minima separated by large barriers. See the Cambridge Cluster Database <http://www-wales.ch.cam.ac.uk/CCD.html> for databases of molecular systems that have been optimized primarily using basin-hopping. This database includes minimization problems exceeding 300 degrees of freedom.