Simulated Annealing

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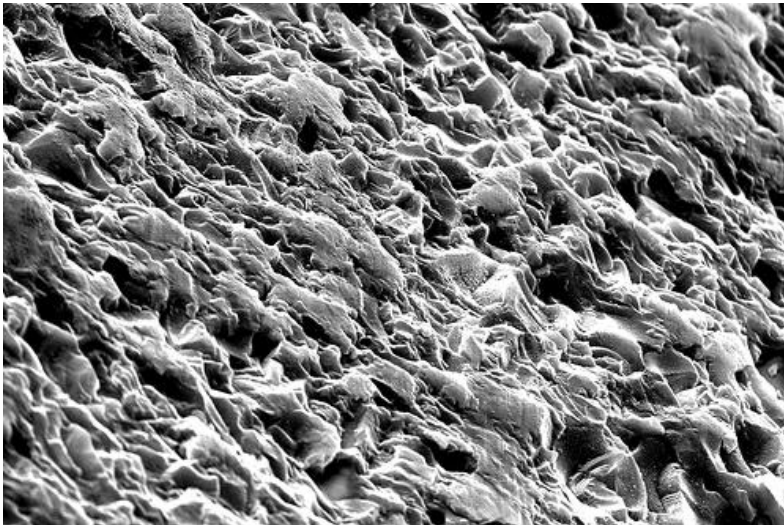Lecturer : Nazlı İkizler Cinbiş

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Content:

- Statistical Mechanics
- NP-Complete Problems
- Heuristics
- Markov Chain
  - Monte Carlo
- Simulated Annealing
  - Implementation Example
  - Strengths-Weaknesses

Statistical Mechanics

- Ever heard Leica?
  - Thousands of $ But WHY?
  - Wetzlar was never bombed during WW2?!!!

Draw a sample crystal view

Statistical Mechanics

- As there are billions of atoms, only the most probable behaviour of them observed in experiments
- Position of an atom is probabilistically;

$$e^{\frac{-\Delta E}{T \times k_B}}$$

  - Where ΔE is the energy change, T is temperature and kB is Boltzmann constant
  - Which means higher the temperature higher the probability range, higher the energy change lower the probability range
- How can one arrange them to form low energy crystal forms?
  - In nature molecules tend to be in a lower energy state. Nature uses the formula above not a linear one

(Kirkpatrick, S.)

NP Complete problems

- Nondeterministic polynomial time problems
- Which can be verified in polynomial time
- Complexity is n^k
- There is not an exact solution but a set of probable solutions.
- Impossible to find with classical search methods.

Heuristics

- Problem specific solutions
- Two strategies
  - Divide and conquer
    - Pieces must be re-arranged after every divide
  - Iterative
    - Search/rearrange until a better configuration is found
    - Usually not to get stuck in local minimums, generate random configurations and save best results globally

Markov Chain

- Next state only depends on the current state
- No Memories!
- Probabilistic approach
- Randomness
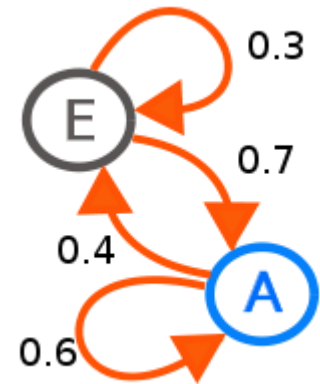
From wiki

Markov Chain Monte Carlo

- Monte Carlo method takes place when the exact solution is not possible to find with deterministic solutions
- Special Markov chain model
- Which has the desire to be in a equilibrium state

Simulated Annealing

- Using thermodynamic rules and statistical mechanics for solving NPC problems with heuristics first introduces in 1953 by Metropolis et al. (Kirkpatric, S. p.2)
- Implemented in 1983 by S. Kirkpatric for solving complex problems; Travelling Salesman and Microprocessor wiring problems
- Actually it is a mixture of all the subjects mentioned in this slideshow earlier.
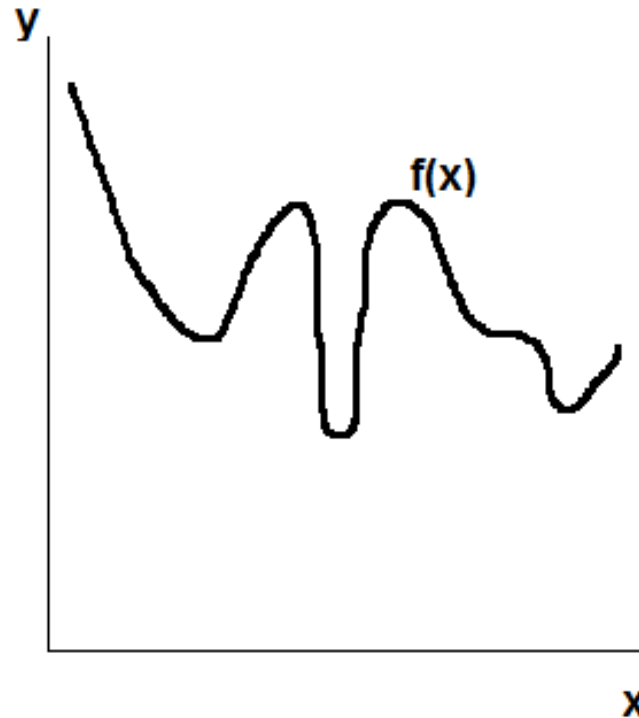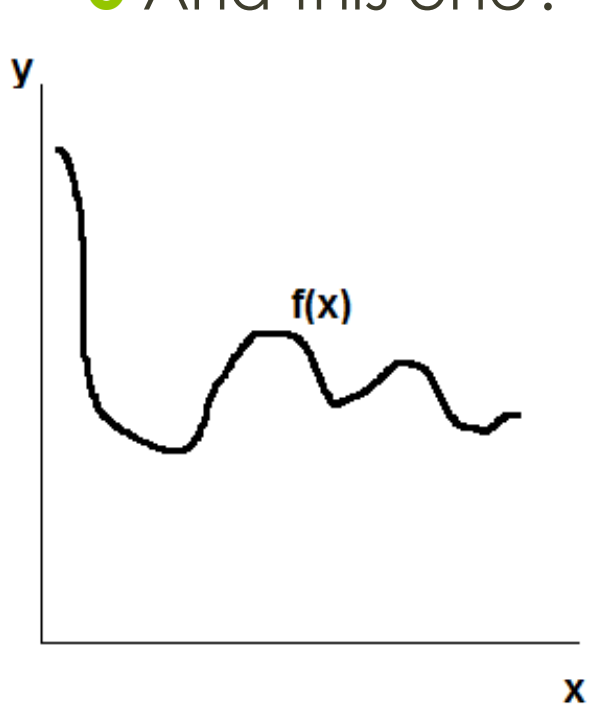
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- Let's have such a decreasing function
- How can we find the global minimum?
  - Increase x slowly and find the minimum y
    - How slowly? How many sampling points?
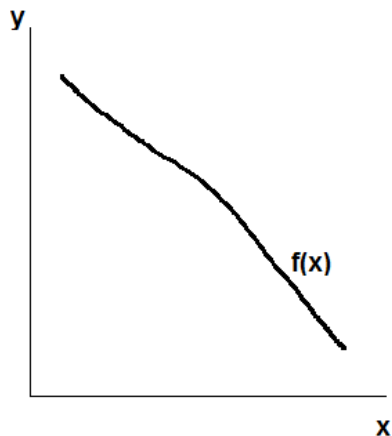
Simulated Annealing

- What about this one?
- And this one?

Simulated Annealing

- Definition : SA is a random search technique which exploits an analogy between the way in which metal cools and freezes into a minimum energy crystalline *(Busetti, F.)*.

- For solving
  - combinatorial minimization problems *(Teukolsky, SA)*
  - NP complete problems *(Teukolsky, SA)*

Simulated Annealing

- Methodology:
- Markov C. Monte C. (take random steps until reaching equilibrium)
  - Starts with an initial state and temperature (analogy from thermodynamics)
  - Randomly changing the state, creates a new state
  - Compares energies of the new state and the current state
  - If the new state has less energy(analogy)
  - OR it's probability function ($e^{\frac{-\Delta E}{T}}$) is less than a random value
    - Accept the new state as the current state
- heuristically iterative and divide-and-conquer (for each temperature creates a new state) by its nature *(Kirkpatrick, S.)*

Simulated Annealing

- The condition below actually accepts a state even if it increases the Energy of the function

- **OR it's probability function ($e^{\frac{-\Delta E}{T}}$) is less than a random value**

- But WHY?
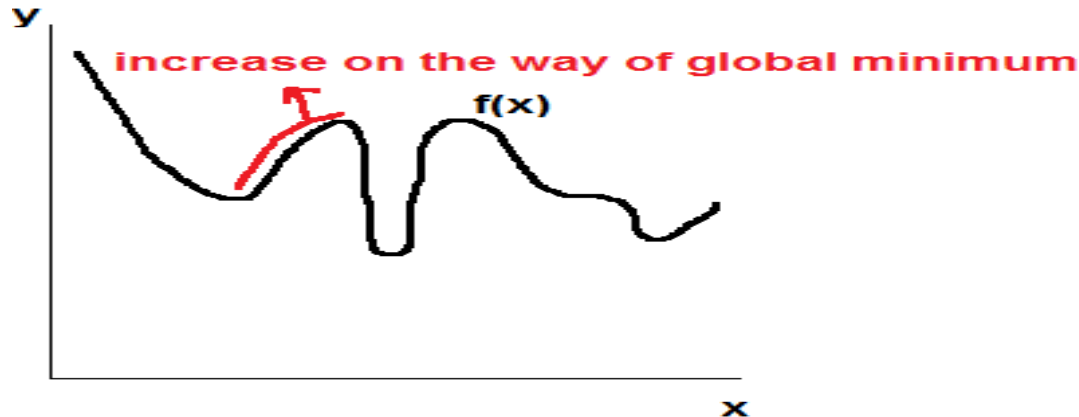
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- Taken from *(Teukolsky, SA, p.445)*
- To make use of the Metropolis algorithm for other than thermodynamic systems, one must provide the following elements:

1. A description of possible system configurations.

2. A generator of random changes in the configuration; these changes are the options" presented to the system.

3. An objective function E (analog of energy) whose minimization is the goal of the procedure.

4. 4. A control parameter T (analog of temperature) and an annealing schedule which tells how it is lowered from high to low values, e.g., after how many random changes in configuration is each downward step in T taken, and how large is that step. The meaning of "high" and "low" in this context, and the assignment of a schedule, may require physical insight and/or trial-and-error experiments.

Simulated Annealing

- Applications
- **Travelling Salesman Problem**
- CODE!

Simulated Annealing

Strengths	Weaknesses
can deal with highly nonlinear models, chaotic and noisy data and many constraints.	Since SA is a metaheuristic, a lot of choices are required to turn it into an actual algorithm.
robust and general technique	There is a clear tradeoff between the quality of the solutions and the time required to compute them
Its main advantages over other local search methods are its flexibility and its ability to approach global optimality.	The tailoring work required to account for different classes of constraints and to fine-tune the parameters of the algorithm can be rather delicate
The algorithm is quite versatile since it does not rely on any restrictive properties of the model	The precision of the numbers used in implementation is of SA can have a significant effect upon the quality of the outcome

(Busetti, F., p.4)

Questions?

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References

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