Traveling Salesman Problem

モデル化とシミュレーション特論
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Sample programs

- https://github.com/modeling-and-simulation-mc-saga/TSP

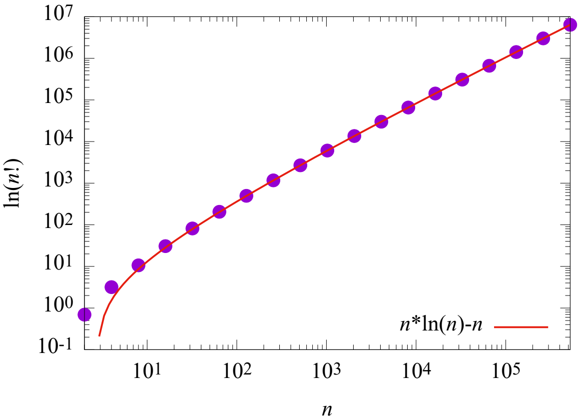
Traveling Salesman Problem

- Given a set of distances $d(c_i, c_j)$ between pairs of N cities
  - Assume the network is complete (any pairs of cities are connected)
  - Set very large values for disconnected pairs
- Find the shortest path, which visits all cities once and comes back to the start.
- Hamiltonian paths
  - Exact method requires to study all possible paths

- The number of possible paths: $(N-1)!/2$
  - Explodes faster than exponential functions for large N
  - Impossible to solve realistic problems in realistic time
- Stirling's formula approximating factorials

$$\ln n! = n \ln n - n + O(\ln n) \tag{1}$$

n	$n!$
1	1
2	2
3	6
4	24
5	120
6	720
7	5040
8	40320
9	362880
10	3628800



Approximate Optimum Solutions

- Do realistic problems require the exact solutions?
  - Obtain good solutions within adequate time available
  - Need methods for obtaining good approximate solutions.

The Nature Can Optimize?

- Crystal growth processes through annealing (徐冷)
  clean crystals through slow cooling down processes
- Structure of proteins
  functional structure through in vivo (生体内) synthesis
- Behavior of ants
  searching shorter paths to feed
- Heredity (遺伝)
  species with higher fitness survive
- Learn approximate optimization from the nature

Optimization in the Nature?

- Search solution space randomly
- Search subspace with good features closely
- very simple
  - how to construct appropriate methods
  - algorithms with random numbers

Simulated Annealing

Simulate slow cooling processes

- finite temperature T
  - Search states (Hamiltonian paths) randomly with transition probabilities specified by T
  - Wide search for high temperature
  - Narrow search for low temperature
  - Monte Carlo Simulation (methods for statistical physics)
- Cooling down gradually
  - Narrow the searching area

Hamilton path and its update

- A close path μ for visiting N cities

$$\mu = \left[c_0^\mu, c_1^\mu, \cdots, c_{N-1}^\mu, c_N^\mu = c_0^\mu\right] \tag{2}$$

- path length

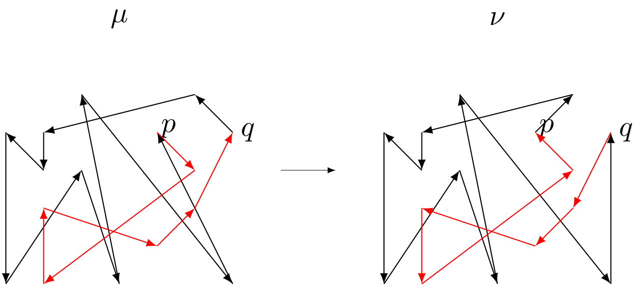
$$D^\mu = \sum_{k=0}^{N-1} d\left(c_k^\mu, c_{k+1}^\mu\right) \tag{3}$$

- Select two points (p, q) in μ randomly

$$\mu = \left[c_0^\mu, c_1^\mu, \cdots, c_{p-1}^\mu, c_p^\mu, c_{p+1}^\mu, \cdots, c_{q-1}^\mu, c_q^\mu, c_{q+1}^\mu, \cdots, c_{N-1}^\mu, c_N^\mu = c_0^\mu\right] \tag{4}$$

- Construct the new close path ν by inverting the path between p and q in μ

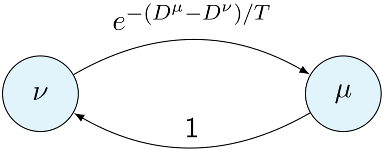
$$\nu = \left[c_0^\mu, c_1^\mu, \cdots, c_{p-1}^\mu, c_q^\mu, c_{q-1}^\mu, \cdots, c_{p+1}^\mu, c_p^\mu, c_{q+1}^\mu, \cdots, c_{N-1}^\mu, c_N^\mu = c_0^\mu\right] \tag{5}$$


μ
p
q
ν
p
q

- if $D^{\nu} < D^{\mu}$
  - Employ the new path ν
  - Obtain shorter path
- if $D^{\nu} \geq D^{\mu}$
  - Employ the new path ν with probability $\exp\left(-\left(D^{\nu} - D^{\mu}\right)/T\right)$
  - Employ longer path with probabilities specified by the temperature

Image of transition between states

- Case $D^\nu < D^\mu$



- For equilibrium

$$e^{-(D^\mu - D^\nu)/T} p(\nu) = p(\mu) \tag{6}$$

probabilities for each close loop

$$p(\mu) \propto e^{-D^\mu/T}, \quad p(\nu) \propto e^{-D^\nu/T} \tag{7}$$

- Repeat trials enough times
- probabilities for each close loop

$$P(\mu) = \frac{1}{Z} \exp\left(-\frac{D^\mu}{T}\right) \tag{8}$$

$$Z = \sum_\mu \exp\left(-\frac{D^\mu}{T}\right) \tag{9}$$

- Z is the normalization constant.
- Z is called partition function, because various statistical quantities can be derived through Z.
- longer paths appear with exponentially low probabilities

Statistical Physics at Finite Temperature

- General frameworks for statistical physics
- System with energy levels $\{E_i\}$
- finite temperature T
- Boltzmann constant k_B, converting temperature to energy

$$P_i = \frac{1}{Z} \exp\left(-\frac{E_i}{k_B T}\right) \tag{10}$$

$$Z = \sum_i \exp\left(-\frac{E_i}{k_B T}\right) \tag{11}$$

Outline of Monte Carlo Simulations

- The current state μ
- Select randomly one of neighboring states$\rightarrow \nu$
- Transit to ν if $E_\nu < E_\mu$
- Otherwise
  - Transit to ν with probability $\exp\left(-\left(E_\nu - E_\mu\right)/T\right)$

Annealing (徐冷)

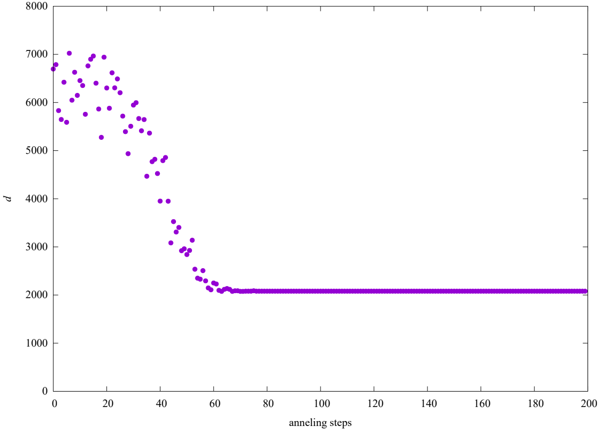
- High temperature
  - Try wide variety of routes
- Lowering temperature slowly
  - Narrow the variety
- Finally the shortest paths can survive

Class Plan: `Route` class

- `List<Point> path`：sequence of nodes
- `double pathLength`：length of the route
- Initialize with some sequence of nodes
- `calcPathLength()`: calculate path length
- `nextRoute()`: generate new path

Class Plan: `Simulation` class

- Change route stochastically
  - `oneMonteCarloStep()`: N trials
  - `oneFlip()`: trial to change route
- Lowering temperature
  - `cooling()`

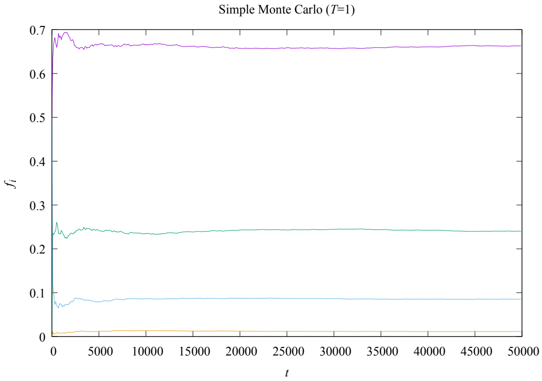

8000
7000
6000
5000
4000
3000
2000
1000
0
d
0
20
40
60
80
100
120
140
160
180
200
anneling steps

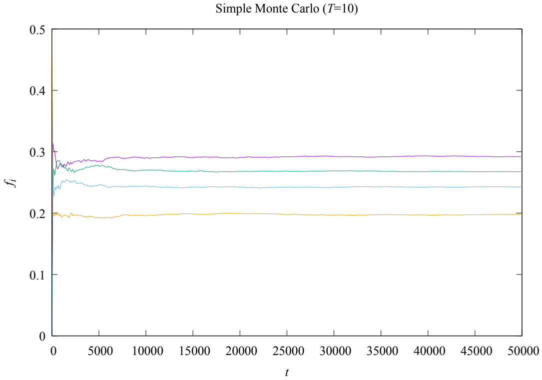
Simple MC Simulation

- Consider n states with energy levels E_i
- Assume any pairs of states connected (transition is possible)
- Set some value of temperature T
- Start from randomly selected state k
- For each step, select randomly one of other state ℓ. And perform state transition.
- Count visits for each state.
- Compute relative frequency of visits.

Example

- $E_i = [0, 1, 2, 4]$
- $T = 1$ and $T = 10$





Equilibrium distributions expected theoretically realise.