Traveling Salesman Problem

モデル化とシミュレーション特論
2023 年度前期
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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 long distance for disconnected pairs
- Find the shortest path, which visits all cities once and comes back to the start.
- Hamiltonian circuits
  - Exact method requires to study all possible circuits
- Example of NP problems

- The number of possible circuits: $(N-1)!/2$

  $N!$

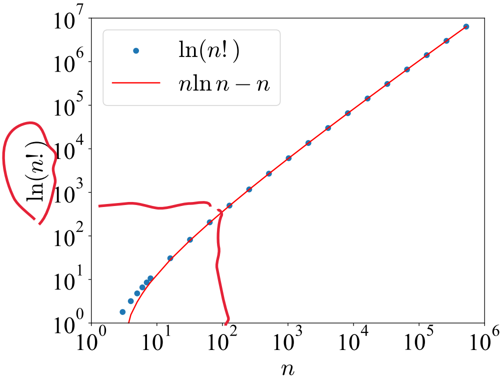
  - Explodes faster than exponential functions for large N
  - Impossible to solve realistic problems in realistic time
- Stirling's formula approximating factorials

$$\ln n! = n \ln n - n + O(\ln n) \tag{1.1}$$

$\ln x = \log_e x$

$\ln n! = \sum_{k=1}^{n} \ln k$

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 closely subspaces with good features
- very simple
    - how to construct appropriate methods
    - algorithms with random numbers

Statistical Physics at Finite Temperature

有限温度の統計力学

- General frameworks for statistical physics
  - General theory for many particle systems
- System with energy levels $\{E_i\}$
- finite temperature T (absolute temperature)
- Boltzmann constant k_B, converting temperature to energy

$$P_i = \frac{1}{Z} \exp\left(-\frac{E_i}{k_B T}\right) \tag{3.1}$$

$$Z = \sum_i \exp\left(-\frac{E_i}{k_B T}\right) \tag{3.2}$$

Partition functions

分配関数

- Z is the normalization constant of the Boltzmann distributions.
- Z is called partition function, because various statistical quantities can be derived through Z. For example:

$$\begin{aligned}\langle E\rangle &= Z^{-1}\sum_i E_i \exp\left(-\frac{E_i}{k_B T}\right) \\ &= k_B T^2 \frac{\partial \ln Z}{\partial T} \qquad (3.3)\end{aligned}$$

- High energy states appear with exponentially low probabilities

Importance Sampling

- How to evaluate $\langle E \rangle$ by simulations?
- Simple Monte Carlo simulation by randomly generating states i will fail.
  - Random sampling fails choosing the dominant states from the huge number of states.
- Importance sampling: sampling states with $p \propto e^{-\beta E_i}$ $(\beta^{-1} = k_B T)$

Outline of Monte Carlo Simulations

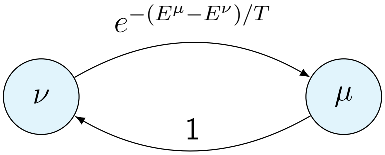
- The current state μ
- Select randomly one of neighboring states$\rightarrow \nu$
- Transit to ν if $E_\nu < E_\mu$
- Otherwise
  - Transit to ν with probability

$$\exp\left(-\frac{E_\nu - E_\mu}{T}\right) \tag{3.4}$$

  - $k_B = 1$ hereafter.

Image of transition between states

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



- For equilibrium

$$e^{-(E^\mu - E^\nu)/T} p(\nu) = p(\mu) \tag{3.5}$$

probabilities for each close loop

$$p(\mu) \propto e^{-E^\mu/T}, \quad p(\nu) \propto e^{-E^\nu/T} \tag{3.6}$$

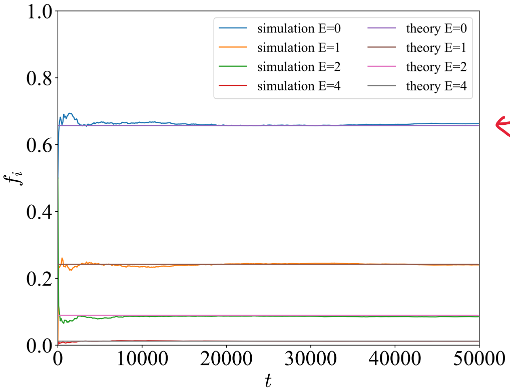
Simple MC Simulation

- 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

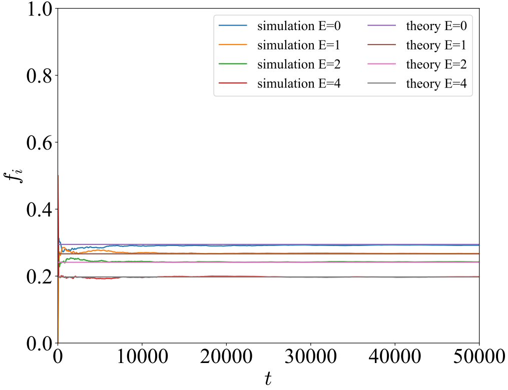
- $E_i = [0, 1, 2, 4]$
- $T = 1$ and $T = 10$

T= 1



$e^{-E_0/T}$

T= 10



Equilibrium distributions expected theoretically realize.

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

$$\mu = \left[c_0^\mu, c_1^\mu, \cdots, c_{N-1}^\mu, c_N^\mu = c_0^\mu\right] \tag{5.1}$$

- path length

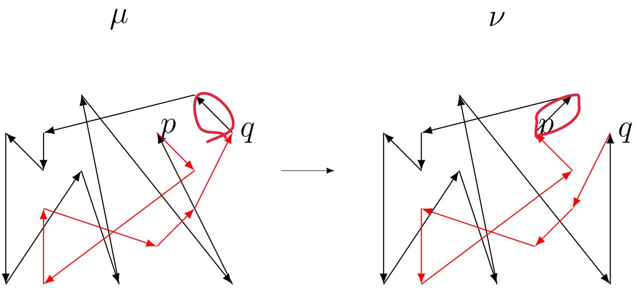
$$D^\mu = \sum_{k=0}^{N-1} d\left(c_k^\mu, c_{k+1}^\mu\right) \tag{5.2}$$

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

$$\mu = \left[c_0^\mu, c_1^\mu, \cdots, c_{p-1}^\mu, c_p^\mu, c_{p+1}^\mu, \cdots, c_{q-1}^\mu, c_q^\mu, c_{q+1}^\mu, \cdots, c_{N-1}^\mu, c_N^\mu = c_0^\mu\right] \tag{5.3}$$

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

$$\nu = \left[c_0^\mu, c_1^\mu, \cdots, c_{p-1}^\mu, c_q^\mu, c_{q-1}^\mu, \cdots, c_{p+1}^\mu, c_p^\mu, c_{q+1}^\mu, \cdots, c_{N-1}^\mu, c_N^\mu = c_0^\mu\right] \tag{5.4}$$


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

$$\exp\left(-\frac{D^\nu - D^\mu}{T}\right) \tag{5.5}$$

  - Employ longer path with probabilities specified by the temperature

Annealing (徐冷)

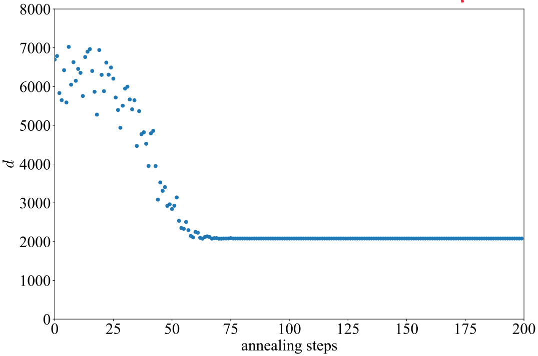
- High temperature
  - Try wide variety of routes
- Lowering temperature slowly
  - Narrow the variety
- Finally the shortest paths can survive

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
25
50
75
100
125
150
175
200
annealing steps