Math 4430

Final Project

Group

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Introduction

Monte Carlo Markov Chain (MCMC) is a method used in statistics and statistical physics to extract sequences of random samples from a probability distribution when direct sampling is difficult. The resulting sequence can be used to estimate the probability distribution or calculate integrals (such as expected values).

MCMC will be used in this report to find a solution to a version of the Travelling Salesman Problem. The Travelling Salesman Problem describes a situation where a salesman must travel to a certain number of cities (in this case 20) without visiting a city more than once. Each of the 20 cities are connected to each other, except for 5 pairs of cities, where travel is forbidden from one city i to another city j. The above circuit where one starts at a city, travels to every other city once, and ends up back at the initial city is also known as a Hamiltonian circuit. Usually, with the Travelling Salesman Problem, the objective is to find the shortest distance that can be travelled in total. However, the problem that is given is to find the average travel time between the 20 cities, or the expected travel time for a circuit chosen from all circuits.

Methodology

The map of cities is described as follows:

- The 20 cities are labelled 1, 2, …, 19, 20.
- Then, five pairs of cities labelled as {i, j} are chosen to have the travel between one city to another city forbidden, meaning that the salesman cannot travel from city i to city j.
    - Note – the assumption when it comes to the pair of cities is that travel is forbidden strictly from city i to city j only, and the pair {i, j} does not work in the converse scenario, meaning travel from city j to city i is not restricted.
- Next, the travel distances between every other pair of cities (185 total) are generated randomly from some distribution on the positive reals that has a density.
    - Note – there are 185 distances that need to be generated. Usually when finding how many paths of travel there are for 20 cities if each city can reach every other city, the number would be $\binom{20}{2}$ = 190 pairs. However, we labelled 5 paths of travel as forbidden, thus removing 5 possible paths and leaving us with 185 travel paths, or 185 pairs of cities.
- Using the metropolis algorithm and taking μ to = 1 (which means we never reject the metropolis algorithm and always jump to the next state), we choose large n and m and sample uniformly from the circuits. Afterwards, we are able to compute the average travel time from this sample.

Before coding, we were tasked with three tasks to answer, two of which related to the metropolis algorithm itself, and one that related to the Q transition matrix of the Travelling Salesman Problem. These will be shown first, followed by the results we have observed from coding the Travelling

Salesman Problem along with the problems we faced.

At the end of this report, the coding used through Python is provided through the Appendix.

Task 1

Write out a proof that P is reversible with respect to μ. Conclude that μ is an invariant probability distribution for P.

Let U be a discrete space continuous time and let μ be a target distribution with all $\mu_i > 0$.

Also let Q be an irreducible transition matrix that is symmetric ($q_{ij} = q_{ji}$) for each i, j.

Also, we have:

$P_{ij} = q_{ij} * \left(1, \frac{\mu_j}{\mu_i}\right)$ $\quad j \neq i$

and

$P_{ij} = 1 - \sum_{k \neq i} \quad q_{ik} * \left(1, \frac{\mu_k}{\mu_i}\right),$ $\quad j = i$

Recall: in a discrete space U, P is reversible with respect to μ if for all i, j: $\mu_i p_{ij} = \mu_j p_{ji}$

We know $\mu_i = \frac{Pi}{\sum_{i=1}^{\infty} \quad Pi}$ where $\sum_{i=1}^{\infty} \quad p_i < \infty$

and similarly, $\mu_j = \frac{Pj}{\sum_{i=1}^{\infty} \quad Pj}$ where $\sum_{i=1}^{\infty} \quad p_j < \infty$

Thus, from what we said above, that

P is reversible with respect to μ if for all i, j: $\mu_i p_{ij} = \mu_j p_{ji}$.

Given P_{ij}, we´ve got 2 cases here: when i = j (case 1) and when i ≠ j (case 2)

Let´s check if the reversibility work for all cases:

<u>Case 1.1:</u> $\frac{\mu_k}{\mu_i} < 1$

$\mu_i p_{ij} = \mu_i * (1 - \sum_{k \neq i} \quad q_{ik} * \frac{\mu_k}{\mu_i}))$

and $\mu_j p_{ji} = \mu_{j*} * (1 - \sum_{k \neq j} \quad q_{jk} * \frac{\mu_k}{\mu_j}))$

As i = j,

$\mu_j p_{ji} = \mu_i * (1 - \sum_{k \neq i} \quad q_{ik} * \frac{\mu_k}{\mu_i})$

Therefore, reversibility works under this condition.

<u>Case 1.2:</u> $\frac{\mu_k}{\mu_i} \geq 1$

$\mu_i p_{ij} = \mu_i * (1 - \sum_{k \neq i} \quad q_{ik*(1)})) = \mu_i p_{ij} = \mu_i * (1 - \sum_{k \neq i} \quad q_{ik})$

and $\mu_j p_{ji} = \mu_j * (1 - \sum_{k \neq i} \quad q_{jk} * 1)) = \mu_j * (1 - \sum_{k \neq j} \quad q_{jk})$

Again, as i = j,

$\mu_j p_{ji} = \mu_j * (1 - \sum_{k \neq i} \quad q_{ik})) = \mu_j * (1 - \sum_{k \neq j} \quad q_{ik})$

Thus, reversibility also works under this condition.

What is left to show that i ≠ j,

<u>Case 2:</u> i ≠ j,

In this case, then the same condition applies, meaning when $\mu_i p_{ij} = \mu_j p_{ji}$.

In other words,

If μ_i*(q_{ij}*min (1, $\frac{\mu_j}{\mu_i}$)) = μ_j*(q_{ji}*min (1, $\frac{\mu_i}{\mu_j}$))

<u>Case 2.1:</u> $\frac{\mu_j}{\mu_i}=1$

Then,

$\mu_i p_{ij} = \mu_i (q_{ij} * 1) = \mu_i * q_{ij}$

$\mu_j p_{ji} = \mu_j * (q_{ji} * 1) = \mu_j * (q_{ji} * 1) = \mu_i * q_{ij}$

Therefore, it is reversible under this condition.

<u>Case 2.2:</u> $\frac{\mu_j}{\mu_i} > 1, \frac{\mu_i}{\mu_j} < 1$

Then,

$\mu_i p_{ij} = \mu_i (q_{ji} * (1)) = \mu_i q_{ij}$

$\mu_j p_{ji} = \mu_j * (q_{ji} * (1)) = \mu_j * (q_{ji} * \frac{\mu_i}{\mu_j}) = \mu_i q_{ij}$ as Q is symmetric.

$\mu_j p_{ji} = \mu_i p_{ij}$

Therefore, it is reversible under this condition too.

<u>Case 2.3:</u> $\frac{\mu_j}{\mu_i} < 1, \frac{\mu_i}{\mu_j} > 1$

Then,

$\mu_i p_{ij} = \mu_i q_{ij} \frac{\mu_j}{\mu_i} = \mu_j q_{ij}$ and

$\mu_j p_{ji} = \mu_j (q_{ji} * (1)) = \mu_j q_{ji} = \mu_i q_{ij} = \mu_i p_{ij}$

Therefore, it is reversible under this condition.

We have shown in all cases that P is reversible with respect to μ.

Hence by this fact, this implies that μ is an invariant probability distribution with respect to P from what we have seen in class concerning the reversibility topic.

Task 2

Now that we have proven the first task, the second task asks us to prove P is irreducible and P is aperiodic when μ is not perfectly uniform.

From the question, we have known that Q is an irreducible transition matrix.

By the definition of irreducibility, for $\forall\, i, j, i \to j$,which means i communicates with j under Q.

We know $P_{ij} = \begin{cases} q_{ij} \min(1, \mu_j/\mu_i) & , i \neq j \\ 1 - \sum_{k\neq i} q_{ik} \min(1, \mu_j/\mu_i) & , i = j \end{cases}$

Since Q is irreducible, then $q_{ij}{}^{(n)} > 0$ for some $n \in Z^+$.

- In the case that $i \neq j$ if $q_{ij}{}^{(n)} > 0$ $P_{ij} = q_{ij} \min(1, \mu_j/\mu_i) > 0$ where $\min(1, \mu_j/\mu_i) > 0$
- In the case that $i = j$ if $q_{ij}{}^{(n)} > 0$, we have
  $$0 < \sum_{k\neq i} q_{ik} \min(1, \mu_j/\mu_i) < 1$$
  $$P_{ij} = 1 - \sum_{k\neq i} q_{ik} \min(1, \mu_j/\mu_i) > 0$$

Hence, $P_{ij}{}^{n} > 0$ for all i, j and P is irreducible, which means $i \to j$ under P.

Since we know that P is irreducible, there is a single equivalence class which means a state can return to itself with one step.

- Suppose μ is perfectly uniform:
  Then $\mu_i = \frac{1}{\Sigma i}\ (i \epsilon S)$

- Suppose μ is not perfectly uniform:
  There exists $\mu_i \neq \mu_j$
  For some i and j, without loss of generality, suppose $\mu_i > \mu_j$
  For the transition from i to j, there is a probability of $p^* = 1 - \frac{\mu_j}{\mu_i}$, where the chain will reject the move from i to j .
  Since $\mu_i > \mu_j$, $p^* = 1 - \frac{\mu_j}{\mu_i} > 0$
  $P_{ii} \geq p^* > 0$
  This period of chain is 1, which means the p is aperiodic.

Task 3

For the Travelling Salesman Problem, task three asks us to check that Q is symmetric.

Q is as follows:

- Let the state space of Q be all the sequences of 20 cities without repetition. Note that some sequences are not valid, as they contain "forbidden trips".
- If i is a sequence above, choose two cities at random, and swap their positions.
  - If the swap creates a sequence with forbidden travel, you would reject the change, and Q will leave the sequence as is.

Note that since the state space of Q is all the sequences of 20 cities (where the cities are labelled 1-20), it can be written as approximately {20!}, and it is close to impossible to write out a matrix that is 20! x 20!. Therefore, we need to write out a written argument that will show that Q can be symmetric.

Consider the following case:

- State i = {1, 2, 3, …, 18, 19, 20}
- State j = {2, 1, 3, …, 18, 19, 20}

Since there is a difference of 2 cities within each state, the probability of moving from state i to state j is $\frac{1}{\binom{20}{2}}$, where $\binom{20}{2}$ =190 is the number of combinations of two cities swapping places.

This means that $q_{ij} = \frac{1}{\binom{20}{2}}$

Since the number of possibilities of choosing two cities to swap is $\binom{20}{2}$, this would also work if we were to move from state j to state i; there would be the same number of possibilities of swapping the position of 2 cities, and the same probability to move back to state i of $\frac{1}{\binom{20}{2}}$. This means that $q_{ji} = \frac{1}{\binom{20}{2}}$ as well, and thus $q_{ij} = q_{ji}$.

Commented [1]: Might need to add what happens when Q leaves the sequence unchanged (ie. when the switch would create a forbidden trip), unless that's also zero

If between state i and state j there is a difference of cities in the sequence that is not two (notably anything above two, since you cannot have one difference), then q_{ij} = 0, since with a single swap of only two cities you could not create two separate sequences that have cities in three or more different positions.

This would also mean that q_{ji} is also 0 with the same logic, since going from state j to state i we would have the same problem of not being able to change the positions of three or more cities with a single swap of two cities.

WLOG, this would happen for all states i and j.

Therefore, since the only possibilities for q_{ij} are 0 or $\frac{1}{\binom{20}{2}}$, and the same probability will happen at q_{ji}, as shown above. This proves that Q is a symmetric matrix.

Task 4

The code is in the appendix to this file.