PURDUE UNIVERSITY · CS 59000-NMC
NETWORKS & MATRIX COMPUTATIONS

LECTURE NOTES
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1 Reversibility in Markov Chains

1.1 Definition

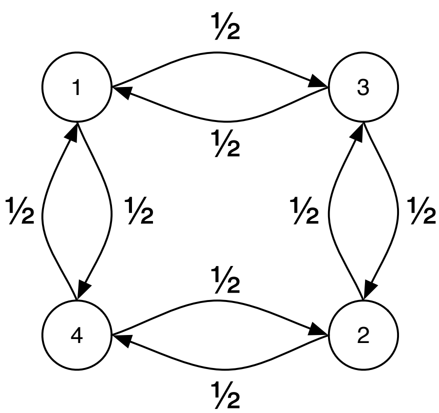
Definition: A process is said to be *reversible* if $(X(n_1), X(n_2), \cdots, X(n_k))$ has the same distribution as $(X(T-n_1), X(T-n_2), \cdots, X(T-n_k))$ for all $n_1, n_2, \cdots, n_k, T \in \mathbb{Z}$, where $X(n_1), X(n_2), \cdots, X(n_k)$ make up the state set.

Result: A Markov chain (MC) is reversible iff there exists $\boldsymbol{\pi}$ such that $\pi_i P_{ij} = \pi_j P_{ji}$, where $\boldsymbol{\pi}$ is the stable distribution. This equation is also called "detailed balance criteria".

Intuitively, $\pi_i P_{ij}$ can be viewed as the probability flux from state i to state j. Thus the detailed balance criteria say that the probability flux from state j to state i equals that from state i to state j. Equivalently, we have the following criterion stating the same thing.

A stationary Markov chain is reversible iff its transition probabilities satisfy $P_{j_1 j_2} P_{j_2 j_3} \cdots P_{j_n j_1} = P_{j_1 j_n} P_{j_n j_{n-1}} \cdots P_{j_2 j_1}$.

Example 1: The following Markov chain is reversible. This example is from here [1].



$$\boldsymbol{P} = \begin{array}{c c} & \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \end{array} & \left(\begin{array}{cc|cc} & & \frac{1}{2} & \frac{1}{2} \\ & & \frac{1}{2} & \frac{1}{2} \\ \hline \frac{1}{2} & \frac{1}{2} & & \\ \frac{1}{2} & \frac{1}{2} & & \end{array}\right) \end{array}$$

Figure 1: A reversible Markov chain and its transition probability matrix $\boldsymbol{P}$

It is easy to see this it is reversible from the equivalent criterion above, since all the transition probabilities are the same. This Markov chain is periodic, which means $\boldsymbol{P}^n$ does not converge. The fact that transition probability matrix $\boldsymbol{P}$ is symmetric is a sufficient condition for reversibility. It is not a necessary condition. From the detailed balance criteria, we have $\pi_i P_{ij} = \pi_j P_{ji}$. If $P_{ij} = P_{ji}$, then we can get the conclusion that $\pi_i = \pi_j$, the uniform distribution. It is obviously that $\pi_i = \dfrac{1}{|S|}$, where $|S|$ is the size of the state set. The stationary distribution is $\boldsymbol{\pi} = (\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4})^T$.

[1] http://www.math.ucsd.edu/~williams/courses/m28908/scullardMath289_Reversibility.pdf

This idea of a symmetric transition Markov for a Markov chain underlies the Markov chain Monte Carlo procedure for sampling complicated objects. We'll see how this works in Example 3.

Example 2: A non-reversible Markov chain. This example is from here [1].

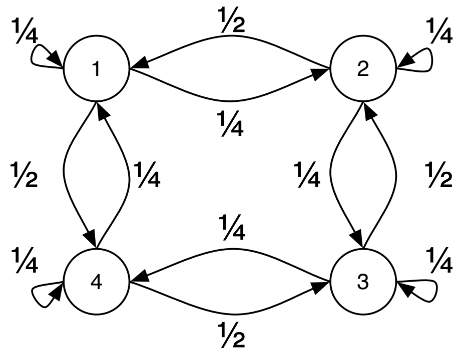


Figure 2: A non-reversible Markov chain

It is easy to see if we walk clockwise, then $P_{13}P_{34}P_{42}P_{21} = (\frac{1}{2})^4 = \frac{1}{16}$. On the other hand, if we walk counterclockwise, then $P_{12}P_{24}P_{43}P_{31} = (\frac{1}{4})^4 = \frac{1}{256}$. Since the two probabilities are not the same, the Markov chain is not reversible. We can also get the stationary distribution $\boldsymbol{\pi}$ by Matlab to show that it fails the $\pi_i P_{ij} = \pi_j P_{ji}$ test.

Given that transition matrix $\boldsymbol{P}$, $\boldsymbol{P}$ is nonnegative and regular. We can get the eigenvalues $\boldsymbol{\lambda}$ and corresponding eigenvectors $\boldsymbol{V}$ of $\boldsymbol{P}^T$. The eigenvalues are $\boldsymbol{\lambda} = (-0.5, 1, 0.25+0.25i, 0.25-0.25i)^T$ and corresponding eigenvectors are as follows. Pick the column corresponding to eigenvalue 1 and normalize the eigenvector, $\boldsymbol{\pi} = (0.25, 0.25, 0.25, 0.25)^T$. It is obvious that $\pi_1 P_{12} = 0.25 \times 0.25 = 0.0625 \neq \pi_2 P_{21} = 0.25 \times 0.5 = 0.125$. This also shows that the Markov chain is not reversible.

$$\boldsymbol{P} = \begin{pmatrix} 0.25 & 0.25 & 0.5 & 0 \\ 0.5 & 0.25 & 0 & 0.25 \\ 0.25 & 0 & 0.25 & 0.5 \\ 0 & 0.5 & 0.25 & 0.25 \end{pmatrix} \qquad \boldsymbol{V} = \begin{pmatrix} -0.5 & 0.5 & 0.5-i & 0.5+i \\ 0.5 & 0.5 & 0.5i & -0.5i \\ 0.5 & 0.5 & -0.5i & 0.5i \\ -0.5 & 0.5 & -0.5 & -0.5 \end{pmatrix}$$

1.2 More examples

Example 3: Permutations.

Consider the Matlab function Randperm. The pseudocode is listed below.

Algorithm 1 Randperm

$p(i) = i, \forall i = 1, 2, \cdots, n$; /* **p** is the permutation vector */
for $k \leftarrow 1, 2, \cdots$ **do**
  Draw i from RandInt$[1, n]$;
  Draw j from RandInt$[1, n]$;
  if $i = j$ **then**
    continue;
  else
    swap $p(i)$ and $p(j)$;
  end if
end for

The algorithm does not allow self loop by if test. An alternative to avoid self loop is to draw (i, j) at the same time with "Draw (i, j) from $\mathsf{RandomPair}((1, n))$". We can view this random permutation problem as a graph problem as follows. The vertex set V is $\mathcal{S}$, where $\mathcal{S}$ is the set of permutations on n things. The edge set is $E = \{(p, q) |\ p$ and q are 1 swap away$\}$. Let us take an example of a permutation on 4 elements.

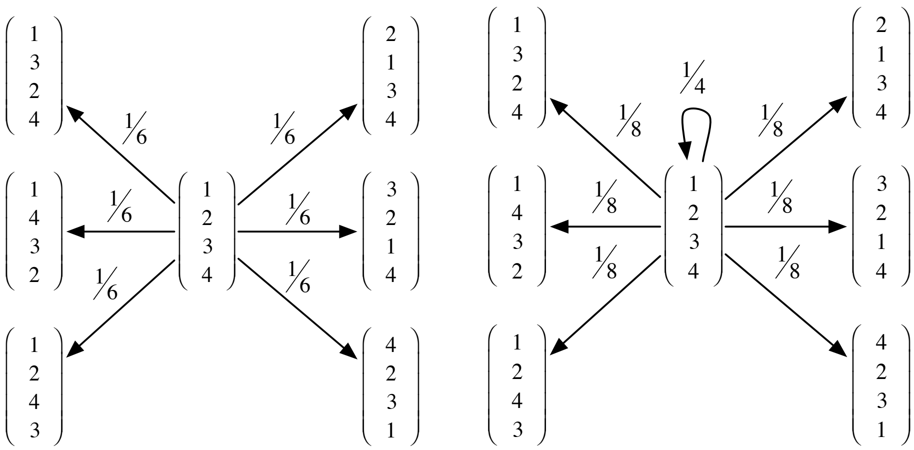
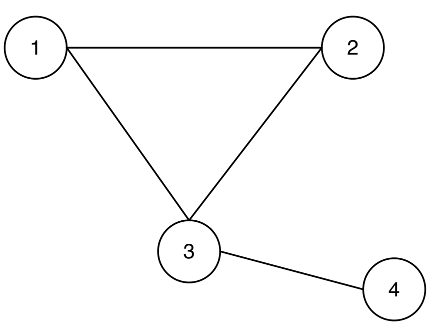


Figure 3: Markov chains on random permutation

If self loop is not allowed in the Markov chain, we can get the figure on the left in Fig. 3. In this case, each state can go to any of the other $\binom{n}{2}$ states. Thus the probability on the edge is $P_{ij} = \frac{1}{\binom{n}{2}}$. However, if selp loop is allowed (as the case shown on the right in Fig. 3), then each state can have n^2 choices now. Therefore, each state has a transition probability of $\dfrac{2}{n^2}$ to other states and the transition probability of $\dfrac{n}{n^2} = \dfrac{1}{n}$ to go back to itself. The algorithm runs like this. Initially, the permutation vector $\mathbf{p} = (1, 2, 3, 4)^T$. On the first iteration, if $(i, j) = (1, 3)$ is chosen, then $\mathbf{p} = (3, 2, 1, 4)^T$. On the second iteration, if $(i, j) = (2, 4)$ is chosen, then $\mathbf{p} = (3, 4, 1, 2)^T$. On the third iteration, if $(i, j) = (3, 2)$, then $\mathbf{p} = (3, 1, 4, 2)^T$, so on and so forth. This algorithm is actually simulating a Markov chain.

Example 4: (uniform) Random walk on an undirected connected graph.



$$P = \begin{array}{c c} & \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \end{array} & \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} \\ 0 & 0 & 1 & 0 \end{pmatrix} \end{array}$$

Figure 4: Random walk on an undirected connected graph

Fig. 4 shows the undirected connected graph and its transition probability matrix. It is easy to see that the transition matrix $\boldsymbol{P}$ can be represented in the following way, $\boldsymbol{P} = \boldsymbol{D}^{-1}\boldsymbol{A}$, where $\boldsymbol{A}$ is the adjacency matrix of the graph and $\boldsymbol{D}$ a diagonal matrix, whose elements are defined as

$$\boldsymbol{D}_{ij} = \begin{cases} deg(i) & \text{if } i = j \\ 0 & \text{else} \end{cases}$$

$\boldsymbol{D}^{-1}$ is actually the diagonal matrix with $\frac{1}{deg(i)}$ on the diagonal. For a weighted graph, $\boldsymbol{D}_{ii} = \sum_{j \in N(i)} w_j \Leftrightarrow \boldsymbol{A}\mathbf{e}$. Given that

$$\boldsymbol{D} = \begin{pmatrix} 2 & & & \\ & 2 & & \\ & & 3 & \\ & & & 1 \end{pmatrix} \qquad \boldsymbol{A} = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

We can verify that $\boldsymbol{P} = \boldsymbol{D}^{-1}\boldsymbol{A}$. The Volume of the graph G is defined as the sum of all the degrees in G. We can find the stationary distribution that makes the Markov chain reversible, where $\pi_i = \dfrac{deg(i)}{Vol(G)}$. The transition matrix $\boldsymbol{P}$ is not symmetric. However the Markov chain is still reversible.

Quiz problem: Let G be an undirected connected graph such that

$$\boldsymbol{P}_{ij} = \begin{cases} 0 & \text{if } (i,j) \notin E \\ \dfrac{d_{\max} - d(i)}{d_{\max}} & \text{if } i = j \\ \dfrac{1}{d_{\max}} & \text{if } (i,j) \in E \end{cases}$$

What is the stationary distribution $\boldsymbol{\pi}$?

Since transition probabilities are all the same, $P_{ij} = P_{ji}$, we can get $\pi_i = \pi_j = \dfrac{1}{n}$.