0.8 Time reversible Markov chains

Consider an ergodic chain $\{\ldots, X_{n-1}, X_n, \ldots\}$ with transition probabilities p_{ij} and stationary distribution π_j. We have

$$p_{ij} = P(X_n = j \,|\, X_{n-1} = i) \tag{102}$$

Now consider the reversed chain, where we run the sequence backwards: $\{\ldots, X_n, X_{n-1}, \ldots\}$. The transition matrix is

$$\begin{aligned} q_{ij} &= P(X_{n-1} = j \,|\, X_n = i) \\ &= \frac{P(X_{n-1} = j, X_n = i)}{P(X_n = i)} \\ &= P(X_n = i \,|\, X_{n-1} = j)\frac{P(X_{n-1} = j)}{P(X_n = i)} \\ &= p_{ji}\,\frac{P(X_{n-1} = j)}{P(X_n = i)} \end{aligned} \tag{103}$$

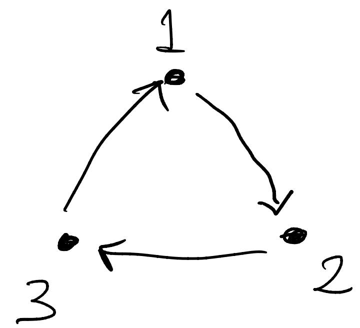
Assume that the original chain is in its stationary distribution so that $P(X_n = i) = \pi_i$ for all i, then this is

$$q_{ij} = p_{ji}\,\frac{\pi_j}{\pi_i} \tag{104}$$

Definition 7 *The Markov chain is* reversible *if $q_{ij} = p_{ij}$ for all $i, j \in S$.*

Markov chain movies played forwards and backwards in time.

Ex. 1 3-state chain



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

Forwards: $1 \to 2 \to 3 \to 1 \to 2 \to 3 \to 1 \to 2 \to 3 \to 1 \to \cdots$

Backwards: $1 \to 3 \to 2 \to 1 \to 3 \to 2 \to 1 \to 3 \to 2 \to \cdots$

Perceptive observer says:

"These look different, so the chain is not time reversible".

<u>More precisely</u>:

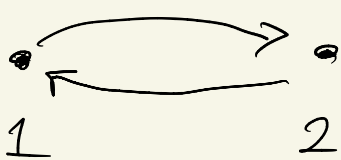
suppose that our observer knows that the transition matrix is

$$P = \begin{array}{cc} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}. & \begin{matrix} 1 \\ 2 \\ 3 \end{matrix} \\ \begin{matrix} 1 & 2 & 3 \end{matrix} & \end{array}$$

Then they can decide with certainty which direction is forward in time.

b/c $1 \to 3$ transition is impossible.

<u>Ex. 2</u> 2-state chain



$$P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Forwards: $1 \to 2 \to 1 \to 2 \to 1 \to 2 \to \cdots$

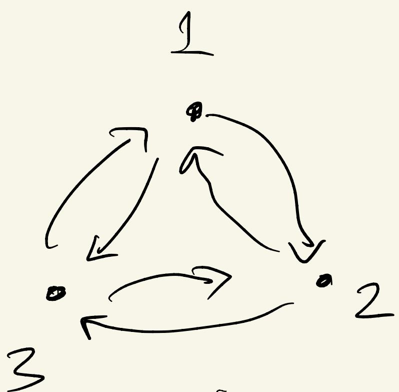
Backwards: $1 \to 2 \to 1 \to 2 \to 1 \to \cdots$

Those are identical.

Observer says "This is the same chain,"

therefore chain is time reversible.

Ex. 3



$$P = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}$$

Forwards: $1 \to 2 \to 3 \to 1 \to 2 \to 3 \to 1 \to 2 \to 3 \to \cdots$

Backwards: $1 \to 3 \to 2 \to 1 \to 3 \to 2 \to 1 \to 3 \to 2 \to \cdots$

Is the chain reversible?

This history is very unlikely, and so it leads to the wrong conclusion, b/c the chain is reversible.

$\Rightarrow$ need an analytical method to decide reversibility.

$$\to X_{n-1} \to X_n \to X_{n+1} \to X_{n+2} \to \cdots$$

$$\leftarrow X_{n-1} \leftarrow X_n \leftarrow X_{n+1} \leftarrow X_{n+2} \leftarrow \cdots$$

<u>Forwards:</u> $$P_{ij} = \mathbb{P}(X_{n+1} = j \mid X_n = i)$$

<u>Backwards:</u> $$q_{ij} = \mathbb{P}(X_n = j \mid X_{n+1} = i)$$

$$= \frac{\mathbb{P}(X_n = j, X_{n+1} = i)}{\mathbb{P}(X_{n+1} = i)}$$

$$= \frac{\mathbb{P}(X_{n+1} = i \mid X_n = j)\, \mathbb{P}(X_n = j)}{\mathbb{P}(X_{n+1} = i)}$$

$$q_{ij} = P_{ji} \frac{\mathbb{P}(X_n = j)}{\mathbb{P}(X_{n+1} = i)}.$$

Assume chain is ergodic (so it has a unique stationary distribution w).

Then

$$\mathbb{P}(X_n = j) \longrightarrow w_j \quad (\text{as } n \to \infty).$$

$\Rightarrow$ reversed chain is

$$\boxed{q_{ij} = P_{ji} \frac{w_j}{w_i}} \quad \text{all } i, j$$

Condition for chain to be <u>reversible</u> is

$$\boxed{q_{ij} = p_{ij}} \quad \text{all states } i, j$$

$$\Longleftrightarrow \quad p_{ji} \frac{w_j}{w_i} = p_{ij}$$

$$\Longleftrightarrow \quad \boxed{w_j p_{ji} = w_i p_{ij}} \quad \text{every } i, j \text{ states}$$

<u>Recall</u>: you computed for ergodic chain

$$\lim_{n \to \infty} \mathbb{P}(X_n = i, X_{n+1} = j)$$

$$= \lim_{n\to\infty} \mathbb{P}(X_{n+1}=j \mid X_n=i)\, \mathbb{P}(X_n=i)$$

$$= P_{ij} \lim_{n\to\infty} \mathbb{P}(X_n=i)$$

$$= w_i P_{ij}$$

= rate of jumps of chain $(i \to j)$.

$$i \longrightarrow j$$

= long-run fraction of jumps from $i \to j$.

Condition for reversibility is

$$W_i P_{ij} = W_j P_{ji}$$

$\Leftrightarrow$ jump rate $(i \to j)$

$=$ jump rate $(j \to i)$.

Why is this useful?

It gives a simpler way to compute W.

The meaning of this equation is that the chain "looks the same" when it is run backwards in time (in its stationary distribution). So you cannot tell whether a movie of the chain is running backwards or forwards in time. Equivalently, for all $i, j \in S$

$$\pi_i p_{ij} = \pi_j p_{ji} \tag{105}$$

The main advantage of this result is that these equations are much easier to solve than the original defining equations for π. There is a nice result which helps here.

Lemma 4 *Consider an irreducible Markov chain with transition probabilities p_{ij}. Suppose there is a distribution $w_j > 0$ such that for all $i, j \in S$*

$$w_i p_{ij} = w_j p_{ji} \tag{106}$$

Then the chain is time reversible and w_j is the stationary distribution.

So this result says that if you can find a positive solution of the simpler equation then you have solved for the stationary distribution.

To see why this is true:

Suppose $w = (w_1, w_2, \dots, w_n)$ satisfies the reversible equations i.e.

$$w_i P_{ij} = w_j P_{ji} \quad \text{all } i, j.$$

Then want to show that

$$\sum_i w_i P_{ij} \overset{?}{=} w_j$$

$$LHS = \sum_i w_i P_{ij} = \sum_i w_j P_{ji}$$

$$= w_j \sum_i P_{ji}$$

row sum of P

$$= w_j \cdot 1$$

$RHS = w_j$ ⟶ equal ⇒ w is the stationary distribution.

Ex. 1

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

Stat. dist. $w = \left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right)$

Check: $w_1 P_{12} \overset{?}{=} w_2 P_{21}$

$\frac{1}{3}(1) \overset{?}{=} \frac{1}{3}(0)$ NO!

Ex 2

$$P = \begin{array}{cc} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & \begin{array}{c} 1 \\ 2 \end{array} \end{array}$$

$w = \left(\frac{1}{2}, \frac{1}{2}\right)$.

Check: $w_i P_{ij} = w_j P_{ji}$ $(i \neq j)$

$w_1 P_{12} \overset{?}{=} w_2 P_{21}$

$\frac{1}{2}(1) = \frac{1}{2}(1)$ $\checkmark$ YES.

chain is reversible.

Ex 3

$$P = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{pmatrix}.$$

$$w = \left(\tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3}\right).$$

$$w_1 P_{12} \stackrel{?}{=} w_2 P_{21}$$

$$\left(\tfrac{1}{3}\right)\left(\tfrac{1}{2}\right) \stackrel{?}{=} \left(\tfrac{1}{3}\right)\left(\tfrac{1}{2}\right) \quad \checkmark$$

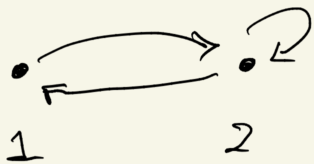
Since w_i is constant, equations become

$$P_{ij} = P_{ji} \iff P = P^T \text{ is symmetric.}$$

True $\Rightarrow$ chain is reversible.

Find stationary distribution by solving reversible equations.

<u>Ex.</u>



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

$$w = (w_1, w_2)$$

solve reversible equations:

$$w_1 P_{12} = w_2 P_{21}$$

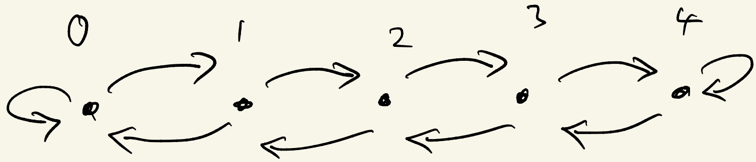
$$w_1 (1) = w_2 \left(\frac{2}{3}\right)$$

$$w_1 = \frac{2}{3} w_2$$

$$w_1 + w_2 = 1.$$

$$\Rightarrow w = \left(\frac{2}{5}, \frac{3}{5}\right).$$

Ex. 2



$$P = \begin{array}{c c} \begin{pmatrix} \frac{1}{3} & \frac{2}{3} & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 0 & \frac{3}{4} & 0 & \frac{1}{4} & 0 \\ 0 & 0 & \frac{1}{5} & 0 & \frac{4}{5} \\ 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix} & \begin{array}{c} 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \end{array}$$

Try to solve reversible equations:

$$w_i P_{ij} = w_j P_{ji}$$

Necessary condition: if $P_{ij} = 0$, must have $P_{ji} = 0$.

Just need to check cases where $P_{ij} \neq 0$.

$$w_0 P_{01} = w_1 P_{10} \Leftrightarrow w_0\left(\frac{2}{3}\right) = w_1\left(\frac{1}{2}\right)$$

$$w_1 P_{12} = w_2 P_{21} \Leftrightarrow w_1\left(\frac{1}{2}\right) = w_2\left(\frac{3}{4}\right)$$

$$w_2 P_{23} = w_3 P_{32} \Leftrightarrow w_2\left(\frac{1}{4}\right) = w_3\left(\frac{1}{5}\right)$$

$$w_3 P_{34} = w_4 P_{43} \Leftrightarrow w_3\left(\frac{4}{5}\right) = w_4\left(\frac{1}{2}\right)$$

$$w_0 + w_1 + w_2 + w_3 + w_4 = 1$$

$$w_1 = \frac{4}{3} w_0$$

$$w_2 = \frac{2}{3} w_1 = \frac{8}{9} w_0$$

$$w_3 = \frac{5}{4} w_2 = \frac{10}{9} w_0$$

$$w_4 = \frac{8}{5} w_3 = \frac{16}{9} w_0$$

$$w_0\left[1 + \frac{12}{9} + \frac{8}{9} + \frac{10}{9} + \frac{16}{9}\right] = 1$$

$$w_0 = \frac{9}{55}$$

$$w_1 = \frac{12}{55}$$

$$w_2 = \frac{8}{55}$$

$$w_3 = \frac{10}{55}$$

$$w_4 = \frac{16}{55}.$$

Example 9 *A total of m white and m black balls are distributed among two boxes, with m balls in each box. At each step, a ball is randomly selected from each box and the two selected balls are exchanged and put back in the boxes. Let X_n be the number of white balls in the first box after n steps. Show that the chain is time reversible and find the stationary distribution.*

If we can solve the time-reversible equations, we are done. The transition matrix is

$$p_{ij} = P(X_1 = j \mid X_0 = i) = \begin{cases} \left(\frac{i}{M}\right)^2 & \text{for } j = i\text{-}1 \\ 2\left(\frac{i}{M}\frac{M-i}{M}\right) & \text{for } j{=}i \\ \left(\frac{M-i}{M}\right)^2 & \text{for } j = i{+}1 \end{cases}$$

Only one time reversible condition needs to be checked:

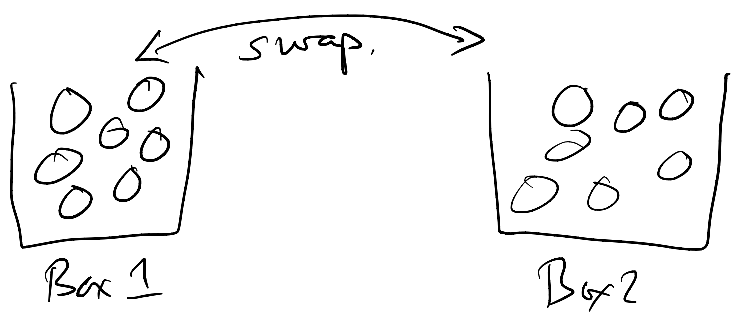
$$\pi_i p_{i,i+1} = \pi_{i+1} p_{i+1,i}$$

in other words

$$\pi_i \left(\frac{M-i}{M}\right)^2 = \pi_{i+1}\left(\frac{i+1}{M}\right)^2$$

Can check that this is satisfied by

$$\pi_i = \frac{\binom{M}{i}^2}{\binom{2M}{M}}$$



m balls

m balls

2m balls
m Black
m White

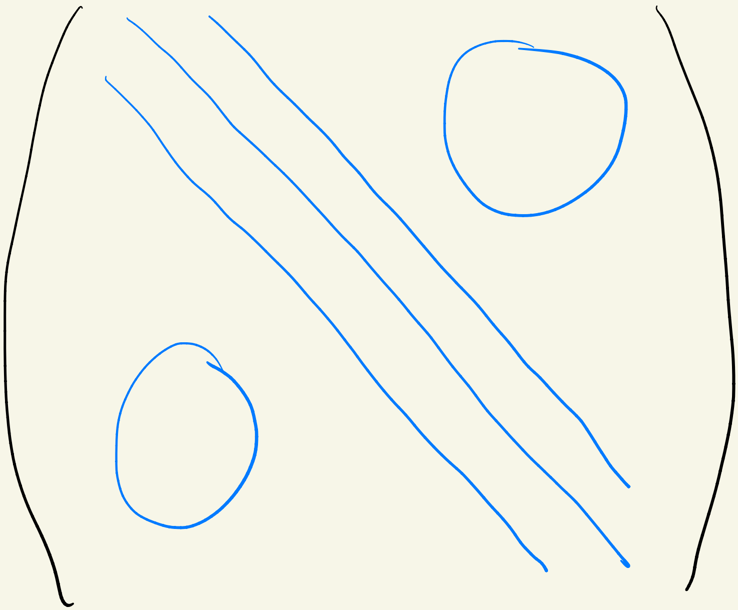
Previously saw example m = 2.

Transition matrix: most entries are zero!

X_n = # Black balls in box 1.

$$X_{n+1} \to \begin{cases} X_n - 1 \\ X_n \\ X_n + 1 \end{cases}$$

only possible changes.

$P =$ 

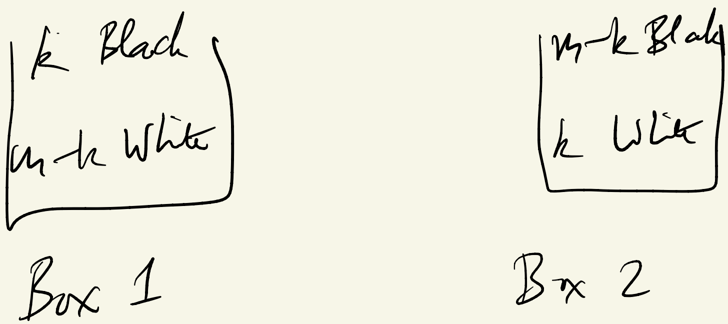
0
1
2
3
⋮
m

$$\mathbb{P}(X_{n+1} = k+1 \mid X_n = k)$$

$= \mathbb{P}($ $k+1$ Black balls $\mid$ k Black balls$)$

$$= \mathbb{P}(\text{choose White in box 1, Black in box 2} \mid X_n = k)$$

$$= \left(\frac{m-k}{m}\right)\left(\frac{m-k}{m}\right) = \left(\frac{m-k}{m}\right)^2.$$



$$P_{k,k+1} = \left(\frac{m-k}{m}\right)^2$$

$$P_{k,k-1} = \left(\frac{k}{m}\right)^2$$

$$P_{k,k} = 2\frac{(m-k)k}{m^2}.$$

Try to solve reversible equations:

$$w_k P_{k,k+1} = w_{k+1} P_{k+1,k}.$$

$$w_k \left(\frac{m-k}{m}\right)^2 = w_{k+1}\left(\frac{k+1}{m}\right)^2.$$

$$\Rightarrow \boxed{w_{k+1} = w_k \left(\frac{m-k}{k+1}\right)^2}$$

Express in terms of w_0.

$$w_1 = w_0\left(\frac{m}{1}\right)^2 = m^2 w_0.$$

$$w_2 = w_1\left(\frac{m-1}{2}\right)^2 = \frac{(m(m-1))^2}{(2)^2} w_0$$

$$W_3 = W_2 \left(\frac{m-2}{3}\right)^2 = W_0 \left(\frac{m(m-1)(m-2)}{(3)(2)(1)}\right)^2$$

$$W_k = W_0 \left(\frac{m(m-1)(m- \quad)(m-k+1)}{k!}\right)^2$$

$$= W_0 \cdot \binom{m}{k}^2 \qquad k=0,1,\dots,m$$

Normalization

$$\sum_{k=0}^{m} W_k = 1$$

$$W_0 \sum_{k=0}^{m} \binom{m}{k}^2 = 1$$

Recall: $$\sum_{k=0}^{m} \binom{m}{k} = 2^m$$

$$\sum_{k=0}^{m} \binom{m}{k}^2 = \binom{2m}{m}.$$

$$\Rightarrow \quad w_k = \frac{\binom{m}{k}}{\binom{2m}{m}} \quad \text{(stationary dist.)}.$$

Therefore:

- chain is reversible
- w is the stationary distribution.

Maybe could have guessed this: this is the probability that a randomly selected set of M balls (drawn from the complete set of $2M$ balls) would contain i white balls and $M - i$ black balls.

The quantity $\pi_i p_{ij}$ has another interpretation: it is the rate of jumps of the chain from state i to state j. More precisely, it is the long-run average rate at which the chain makes the transition between these states:

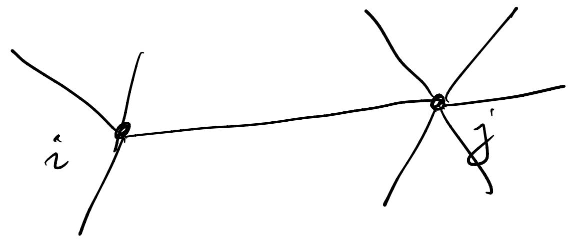
$$\lim_{n\to\infty} P(X_n = i\,,\, X_{n+1} = j) = \pi_i p_{ij} \tag{107}$$

This often helps to figure out if a chain is reversible.

Example 10 *Random walk on graph.*

$P_{ij} = \frac{1}{4}$

$P_{ji} = \frac{1}{6}$



Graph: vertices and edges (not directed).

Random walk:

X_n = position after n steps is a vertex on graph.

Jump: X_{n+1} : randomly choose an edge at X_n, and jump along it.

Try to solve reversible equations

$$w_i P_{ij} = w_j P_{ji}$$

$$\boxed{w_i \frac{1}{d_i} = w_j \frac{1}{d_j}}$$

d_i = degree of vertex i

= # edges at i

solution: $w_i = c\, d_i$ some constant c.

$$\boxed{w_i = d_i / \sum_j d_j}$$