STAT253/317 Lecture 6 Time Reversibility (§4.8)

4.8.1 Backward Markov Chain

If $\{\ldots, X_{n-1}, X_n, X_{n+1}, \ldots\}$ is a Markov chain, the backward chain $\{\ldots, X_{n+1}, X_n, X_{n-1}, \ldots\}$ is also a Markov chain.

Proof.

$$
\begin{aligned}
&\mathrm{P}(X_m = j \mid X_{m+1} = i, X_{m+2}, X_{m+3}, \ldots) \\
&= \frac{\mathrm{P}(X_m = j, X_{m+1} = i, X_{m+2}, X_{m+3}, \ldots)}{\mathrm{P}(X_{m+1} = i, X_{m+2}, X_{m+3}, \ldots)} \\
&= \frac{\boxed{\mathrm{P}(X_{m+2}, X_{m+3}, \ldots \mid X_m = j, X_{m+1} = i)}\mathrm{P}(X_m = j, X_{m+1} = i)}{\mathrm{P}(X_{m+2}, X_{m+3}, \ldots \mid X_{m+1} = i)\mathrm{P}(X_{m+1} = i)} \\
&= \frac{\mathrm{P}(X_{m+2}, X_{m+3}, \ldots \mid X_{m+1} = i)\mathrm{P}(X_m = j, X_{m+1} = i)}{\mathrm{P}(X_{m+2}, X_{m+3}, \ldots \mid X_{m+1} = i)\mathrm{P}(X_{m+1} = i)} \quad \text{(Markov Property}\\
&= \frac{\mathrm{P}(X_m = j, X_{m+1} = i)}{\mathrm{P}(X_{m+1} = i)} = \mathrm{P}(X_m = j \mid X_{m+1} = i)
\end{aligned}
$$

Transition Probabilities of the Backward Markov Chain

Consider a Markov chain $\{X_n : n = 0, 1, 2, \ldots\}$ with transition probabilities $\{P_{ij}\}$.

Let $\{\pi_j^{(m)} = P(X_m = j)\}$ be the marginal distribution of X_m.

The transition probabilities $\{Q_{ij}^{(m)}\}$ of the backward Markov chain are

$$
\begin{aligned}
Q_{ij}^{(m)} &= \mathrm{P}(X_m = j \mid X_{m+1} = i) \\
&= \frac{\mathrm{P}(X_m = j, X_{m+1} = i)}{\mathrm{P}(X_{m+1} = i)} \\
&= \frac{\mathrm{P}(X_m = j)\mathrm{P}(X_{m+1} = i \mid X_m = j)}{\mathrm{P}(X_{m+1} = i)} = \frac{\pi_j^{(m)} P_{ji}}{\pi_i^{(m+1)}}
\end{aligned}
$$

We can see the backward Markov chain is **NOT stationary** because the transition probabilities $Q_{ij}^{(m)}$ depend on m.

To make the backward Markov chain **stationary**, the forward chain must start with its stationary distribution $\{\pi_j\}$ so that

$$P(X_m = j) = \pi_j \quad \text{for all } m$$

the transition probabilities $\{Q_{ij}\}$ of the backward Markov chain is

$$\begin{aligned} Q_{ij} &= \mathrm{P}(X_m = j \mid X_{m+1} = i) \\ &= \frac{\mathrm{P}(X_m = j, X_{m+1} = i)}{\mathrm{P}(X_{m+1} = i)} \\ &= \frac{\mathrm{P}(X_m = j)\mathrm{P}(X_{m+1} = i \mid X_m = j)}{\mathrm{P}(X_{m+1} = i)} = \frac{\pi_j P_{ji}}{\pi_i} \end{aligned}$$

which does not depend on m

Time Reversible Markov Chains & Detailed Balanced Equations

A Markov chain is said to be *time reversible* iff

$$Q_{ij} = P_{ij},$$

i.e., **it behaves exactly the same** no matter **running forward or backward** when in the stationary state.

Because Q_{ij} equals $\pi_j P_{ji}/\pi_i$, a Markov chain is time reversible if and only if its stationary distribution $\{\pi_j\}$ satisfies the equations

$$\pi_i P_{ij} = \pi_j P_{ji} \quad \text{for all } i, j.$$

This set of equations is called the **detailed balanced equation**.

Balanced Equations v.s. Detailed Balanced Equations

Recall a distribution π_j for a Markov chain is said to be stationary if and only if it satisfies

$$\pi_j = \sum_{i \in \mathfrak{X}} \pi_i P_{ij} \quad \text{for all } j \in \mathfrak{X}.$$

This set of equations is called the **balanced equations**.

Balanced Equations v.s. Detailed Balanced Equations

Recall a distribution π_j for a Markov chain is said to be stationary if and only if it satisfies

$$\pi_j = \sum_{i \in \mathfrak{X}} \pi_i P_{ij} \quad \text{for all } j \in \mathfrak{X}.$$

This set of equations is called the **balanced equations**.

A solution to the **detailed balanced equations** must also be a solution to the **balanced equations**, because

$$\sum\nolimits_{i \in \mathfrak{X}} \pi_i P_{ij} = \sum\nolimits_{i \in \mathfrak{X}} \pi_j P_{ji} = \pi_j \sum\nolimits_{i \in \mathfrak{X}} P_{ji} = \pi_j \cdot 1 = \pi_j$$

Balanced Equations v.s. Detailed Balanced Equations

Recall a distribution π_j for a Markov chain is said to be stationary if and only if it satisfies

$$\pi_j = \sum_{i \in \mathfrak{X}} \pi_i P_{ij} \quad \text{for all } j \in \mathfrak{X}.$$

This set of equations is called the **balanced equations**.

A solution to the **detailed balanced equations** must also be a solution to the **balanced equations**, because

$$\sum\nolimits_{i \in \mathfrak{X}} \pi_i P_{ij} = \sum\nolimits_{i \in \mathfrak{X}} \pi_j P_{ji} = \pi_j \sum\nolimits_{i \in \mathfrak{X}} P_{ji} = \pi_j \cdot 1 = \pi_j$$

It is possible that the balanced equations have solutions but the detailed balanced equations do not.

Interpretation of the Balanced Equation

$$
\begin{aligned}
\pi_j &= \sum_{i \in \mathfrak{X}} \pi_i P_{ij} \quad \text{for all } j \in \mathfrak{X} \\
\Leftrightarrow \quad \pi_j(1 - P_{jj}) &= \sum_{i \in \mathfrak{X}, i \neq j} \pi_i P_{ij} \quad \text{for all } j \in \mathfrak{X}
\end{aligned}
$$

$$\boxed{\text{rate of transitions } \textbf{out of} \text{ state } j = \text{rate of transitions } \textbf{into} \text{ state } j}$$

$$
\begin{array}{ccccc}
 & \bullet & \bullet & \bullet & \\
 & \nwarrow & \uparrow & \nearrow & \\
\bullet & \longleftarrow & j & \longrightarrow & \bullet \\
 & \swarrow & \downarrow & \searrow & \\
 & \bullet & \bullet & \bullet &
\end{array}
\qquad\qquad
\begin{array}{ccccc}
 & \bullet & \bullet & \bullet & \\
 & \searrow & \downarrow & \swarrow & \\
\bullet & \longrightarrow & j & \longleftarrow & \bullet \\
 & \nearrow & \uparrow & \nwarrow & \\
 & \bullet & \bullet & \bullet &
\end{array}
$$

How many equations are there in the Balanced euqations?
# of balanced equations = # of states

Interpretation of the Detailed Balanced Equation

Detailed balanced equations are easier to solve but
there might not be a solutions

Balanced equations are more difficult to solve but more
likely to have a solutions.

$$\pi_i P_{ij} = \pi_j P_{ji}$$

$$\boxed{\text{rate of transitions from } i \text{ to } j = \text{rate of transitions from } j \text{ to } i}$$

$$i \longrightarrow j \qquad\qquad j \longrightarrow i$$

How many detailed balanced equations are there in total?

Ans: # of equations = number of pairs of states
If there are N states, there are N(N-1)/2 equations

How many unknowns are there?
Ans: # of states = N

Example 4.35

Consider a random walk with states $0, 1, \ldots, M$ and transition probabilities

$$\begin{aligned} P_{i,i+1} &= \alpha_i = 1 - P_{i,i-1}, \quad \text{for } i = 1, \ldots, M-1, \\ P_{0,1} &= \alpha_0 = 1 - P_{0,0}, \\ P_{M,M} &= \alpha_M = 1 - P_{M,M-1} \end{aligned}$$

$$0 \xrightarrow{\alpha_0} 1 \xrightarrow{\alpha_1} 2 \cdots \longrightarrow M-1 \xrightarrow{\alpha_{M-1}} M \overset{\alpha_M}{\circlearrowleft}$$

1-alpha2

$$\overset{1-\alpha_0}{\circlearrowleft}\ 0 \xleftarrow{1-\alpha_1} 1 \xleftarrow{\alpha_2} 2 \cdots \longrightarrow M-1 \xleftarrow{1-\alpha_M} M$$

Example 4.35 (Cont'd)

The stationary distribution π can be solved via the detailed balanced equation

$$\pi_i P_{i,i-1} = \pi_i(1-\alpha_i) = \pi_{i-1} P_{i-1,i} = \pi_{i-1}\alpha_{i-1}$$

So

$$\pi_i = \frac{\alpha_{i-1}}{1-\alpha_i}\pi_{i-1} = \ldots = \frac{\alpha_{i-1}\alpha_{i-2}\ldots\alpha_0}{(1-\alpha_i)(1-\alpha_{i-1})\ldots(1-\alpha_1)}\pi_0$$

Since $\sum_0^M \pi_i = 1$, one can solve π_0 via

$$\pi_0\left[1+\sum\nolimits_{i=1}^{M}\frac{\alpha_{i-1}\alpha_{i-2}\ldots\alpha_0}{(1-\alpha_i)(1-\alpha_{i-1})\ldots(1-\alpha_1)}\right] = 1$$

A Non-Time-Reversible Markov Chain

In Exercise 4.34 (a flea moving around the vertices of a triangle),

$$\begin{tikzcd} & 1 \arrow[dr, "p_1"] & \\ 3 \arrow[ur, "p_3"] & & 2 \arrow[ll, "p_2"'] \end{tikzcd} \qquad \begin{tikzcd} & 1 \arrow[dl, "q_1"'] & \\ 3 \arrow[rr, "q_3"] & & 2 \arrow[ul, "q_2"'] \end{tikzcd} \qquad \text{where } p_i + q_i = 1$$

the transition probabilities, and the stationary distribution are respectively

$$\begin{array}{cc} & \begin{array}{ccc} 1 & 2 & 3 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \end{array} & \begin{pmatrix} 0 & p_1 & q_1 \\ q_2 & 0 & p_2 \\ p_3 & q_3 & 0 \end{pmatrix} \end{array}, \quad \text{and } \pi = \left(\frac{1 - p_2 q_3}{C}, \frac{1 - p_3 q_1}{C}, \frac{1 - p_1 q_2}{C}\right)$$

where $C = 3 - p_2 q_3 - p_3 q_1 - p_1 q_2$. One can easily verify that

$$\pi_1 P_{12} = \pi_1 p_1 \neq \pi_2 P_{21} = \pi_2 q_2$$

The chain is NOT time reversible.

Other Non-Time-Reversible Markov Chains

- A Markov chain with **transient states** cannot be time-reversible because then running forward and backward in time will not be equivalent.

- If there exists two states i and j such that

$$P_{ij} > 0 \quad \text{but} \quad P_{ji} = 0$$

then the Markov chain cannot be time-reversible because then when running backward in time

$$Q_{ij} = \frac{\pi_j P_{ji}}{\pi_i} = 0 \neq P_{ij}.$$

Theorem 4.2

An ergodic Markov chain for which $P_{ij} = 0$ whenever $P_{ji} = 0$ is time reversible if and only if starting in state i, any path back to i has the same probability as the reversed path. That is, if

$$P_{ii_1} P_{i_1 i_2} \dots P_{i_k i} = P_{ii_k} P_{i_k i_{k-1}} \dots P_{i_1 i}$$

for all states $i, i_1, \dots, i_k$.

$$\begin{tikzcd}
 & i_k \arrow[r] & i \arrow[dr] & \\
i_{k-1} \arrow[ur] & & & i_1 \arrow[dl] \\
 & \cdots \arrow[ul] & i_2 \arrow[l] &
\end{tikzcd}
\qquad
\begin{tikzcd}
 & i_k \arrow[dl] & i \arrow[l] & \\
i_{k-1} \arrow[dr] & & & i_1 \arrow[ul] \\
 & \cdots \arrow[r] & i_2 \arrow[ur] &
\end{tikzcd}$$

For some ergodic Markov chains that have no cycles, like 1-D random walk, they must be time-reversible

Theorem 4.2 — Proof of Necessity

If a Markov chain is time reversible, we have

$$\pi_i P_{ij} = \pi_j P_{ji}, \quad \pi_k P_{kj} = \pi_j P_{jk}.$$

implying (if $P_{ij} P_{jk} > 0$) that

$$\frac{\pi_i}{\pi_k} = \frac{P_{ji} P_{kj}}{P_{ij} P_{jk}},$$

but $\pi_i P_{ik} = \pi_k P_{ki}$ also implies $\pi_i / \pi_k = P_{ki} / P_{ik}$. Thus

$$P_{ik} P_{kj} P_{ji} = P_{ij} P_{jk} P_{ki}.$$

This proves for the case $i \to j \to k \to i$. The general case for longer cycle can be proved similarly

Theorem 4.2 — Proof of Sufficiency

Consider the cycle $i \to i_1 \to i_2 \to \ldots \to i_k \to j \to i$.

$$P_{ii_1} P_{i_1 i_2} \ldots P_{i_k j} P_{ji} = P_{ij} P_{ji_k} P_{i_k i_{k-1}} \ldots P_{i_1 i}$$

Summing the preceding over all states $\cancel{i,}\, i_1, \ldots, i_k$ yields

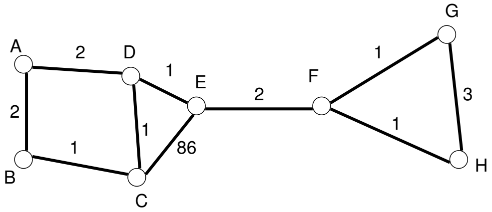
$$P_{ij}^{(k \cancel{+1})} P_{ji} = P_{ij} P_{ji}^{(k \cancel{+1})}$$

Letting $k \to \infty$ yields

$$\pi_j P_{ji} = P_{ij} \pi_i$$

which proves the theorem.

Example 4.36 Random Walk on a Weighted Graph (p.241)



A graph = a set of vertices (or nodes) + a set of arcs (or edges) connecting some pairs of vertices. We consider random walk on a connected graph such that

- each pair (i, j) of vertices are connected by at most one arc;
- all arcs are undirected: arc $(i, j) =$ arc (j, i);
- there is a path consists of arcs connecting any pair of vertices;
- each arc (i, j) is associated with a weight $w_{ij} > 0$
    - $w_{ij} = 0$ if there is not arc connecting (i, j)
    - $w_{ij} = w_{ji}$

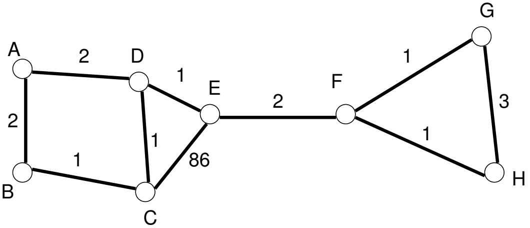
Example 4.36 Random Walk on a Weighted Graph (p.241)

A particle moving from vertices to vertices that if at any time the particle is at node i, then it will next move to node j with probability

$$P_{ij} = \frac{w_{ij}}{\sum_k w_{ik}},$$

E.g., in the graph below, there are two arcs from vertices B with weights $w_{BA} = 2$ and $W_{BC} = 1$ respectively. So,

$$P_{BA} = \frac{w_{BA}}{w_{BA} + w_{BC}} = \frac{2}{2+1} = \frac{2}{3}, \quad P_{BC} = \frac{w_{BC}}{w_{BA} + w_{BC}} = \frac{1}{2+1} = \frac{1}{3}.$$



Random walk on a graph is **irreducible** because the graph is **connected**.

Random Walk on a Weighted Graph is Time Reversible

Solving the detailed balanced equation:

$$\pi_i P_{ij} = \frac{\pi_i w_{ij}}{\sum_k w_{ik}} = \frac{\pi_j w_{ji}}{\sum_k w_{jk}} = \pi_j P_{ji} \quad \text{for all } i, j$$

or, equivalently, since $w_{ij} = w_{ji}$,

$$\frac{\pi_i}{\sum_k w_{ik}} = \frac{\pi_j}{\sum_k w_{jk}} \quad \text{for all } i, j,$$

which means $\frac{\pi_i}{\sum_k w_{ik}}$ is a constant c for all i, i.e.,

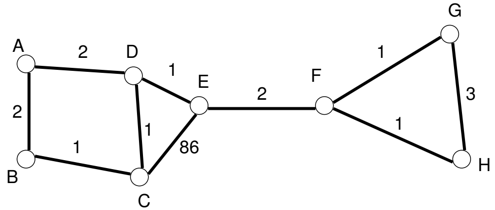
$$\pi_i = c \sum_k w_{ik}.$$

Since $1 = \sum_j \pi_j = c \sum_j \sum_k w_{jk}$, we know $c = 1/(\sum_j \sum_k w_{jk})$, and hence

$$\pi_i = \frac{\sum_k w_{ik}}{\sum_j \sum_k w_{jk}}$$

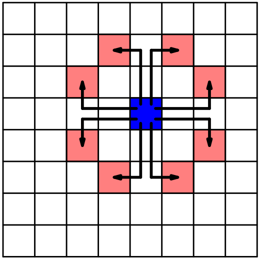
is a solution to the detailed balanced eq. The process is therefore time-reversible.

Random Walk on a Weighted Graph

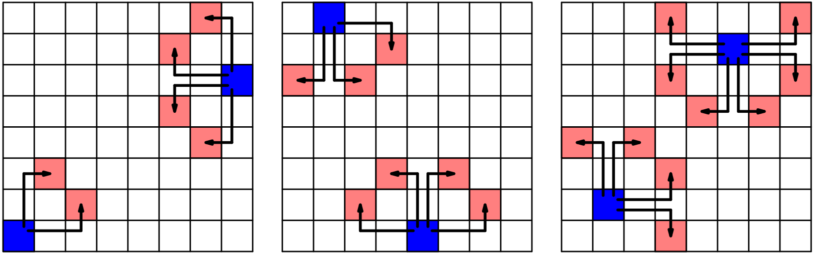


Vertices i	$\sum_k w_{ik}$	π_i
A	$2+2=4$	$\pi_A = 4/200$
B	$2+1=3$	$\pi_B = 3/200$
C	$1+1+86=88$	$\pi_C = 88/200$
D	$2+1+1=4$	$\pi_D = 4/200$
E	$1+2+86=89$	$\pi_E = 89/200$
F	$2+1+1=4$	$\pi_F = 4/200$
G	$1+3=4$	$\pi_G = 4/200$
H	$1+3=4$	$\pi_H = 4/200$
Sum	$\sum_i \sum_k w_{ik} = 200$	

Random Knight on a Chessboard

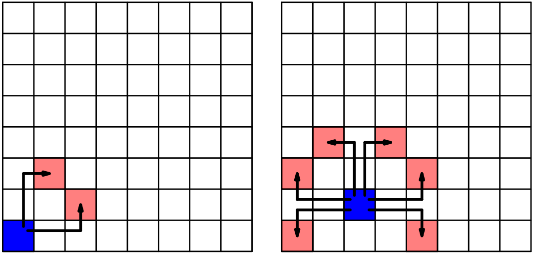


- The Knight moves in an **L** shape in any direction.
- At the blue square, the Knight can move to any of the 8 red squares.
- From a square near the boundary, the Knight has fewer possible moves as it cannot move out of the Chessboard (see the 3 graphs below.)



Random Knight on a Chessboard

- A Knight moves randomly on an empty chessboard.
- In each step, it's equally like to take any of its legal moves. E.g., at the corner, it has prob. $1/2$ each to move to either of the two red squares, from which it has prob. $1/6$ each to move to any of the 6 possible squares.



- Each move is indep. of the history of moves up to that time.
- The position of on knight after nth move is a Markov chain where states are the 64 squares on the chessboard.

Random Knight on a Chessboard

The Knight's random walk on a Chessboard is also a random walk on weighted graph where

- the vertices are the 64 squares on the chessboard;
- there is an arc between any two squares that Knight can move in 1 step;
- all the arcs have weight $w_{ij} = 1$.

The transition probability of a random walk on weighted graph from square i to square j is

$$\begin{aligned} P_{ij} = \frac{w_{ij}}{\sum_k w_{ik}} &= \frac{1}{\#\text{ of squares that connected with square } i \text{ with an arc}} \\ &= \frac{1}{\#\text{ of legal moves from square } i} \end{aligned}$$

which is exactly the random walk of the knight.

Random Knight on a Chessboard

Using the property of random walks on a graph, the stationary distribution of the Knight's random walk is

$$\pi_i = \frac{\sum_k w_{ik}}{\sum_j \sum_k w_{jk}} = \frac{\text{\# of legal moves from square } i}{\sum_j (\text{\# of legal moves from square } j)}$$

The numbers of legal moves from the squares are as follows:

2	3	4	4	4	4	3	2
3	4	6	6	6	6	4	3
4	6	8	8	8	8	6	4
4	6	8	8	8	8	6	4
4	6	8	8	8	8	6	4
4	6	8	8	8	8	6	4
3	4	6	6	6	6	4	3
2	3	4	4	4	4	3	2

The sum of the number of possible moves over all squares is

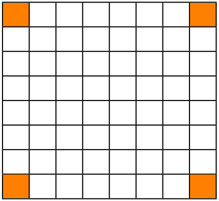
$$2 \times 4 + 3 \times 8 + 4 \times 20$$
$$+ 6 \times 16 + 8 \times 16 = 336.$$

The long run proportion of time that the Knight is in a specific square is simply the counts in the table above divided by 336.

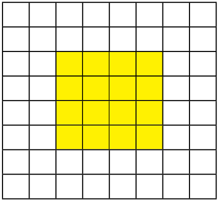
Return Time of a Random Knight

Recall that $1/\pi_i = \mathbb{E}[T_i]$ is the expected time between two visits of the Markov chain to state i.

Starting from one of the four corners, it takes $1/\pi_i = 336/2 = 168$ moves on average for a Knight to return to its initial position.



Starting from the center of the chessboard, it takes $1/\pi_i = 336/8 = 42$ moves on average for a Knight to return to its initial position



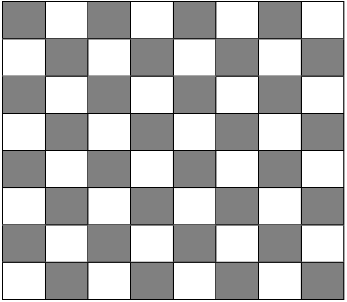
More Questions

- Is this Markov chain irreducible? That is, can the Knight visit every square from every square?

- What is the period of this Markov chain?

More Questions

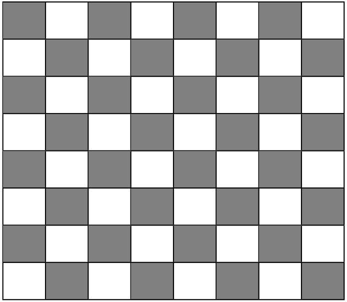
- Is this Markov chain irreducible? That is, can the Knight visit every square from every square?
- What is the period of this Markov chain?



More Questions

- Is this Markov chain irreducible? That is, can the Knight visit every square from every square?

- What is the period of this Markov chain?



Every "L" move can only from a gray square to a white square or a white square to a gray square.