# The Long Run Behavior of Markov Chains (Chapter 10)

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Stats 102C: Introduction to Monte Carlo Methods

## UCLA

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Acknowledgements: Qing Zhou

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• Consider a two-state Markov chain, with state space  $\{0,1\}$  and transition matrix

$$\mathbb{P} = \begin{bmatrix} 0.8 & 0.2 \\ 0.3 & 0.7 \end{bmatrix}.$$

- Suppose we are given that the chain starts at 0:  $X_0 = 0$ .
- We want to generate  $X_1, X_2, \ldots, X_n$ , for some large n (for example, n = 10000).
- Goal:

long van

- How often is the Markov chain in state 0?
- How often is the Markov chain in state 1?

R Code to generate two-state Markov chain:

```
> set.seed(9999) # for reproduceability
             times
> n <- 10000 # specify length of chain
> # Specify transition matrix
> P <- rbind(c(0.8, 0.2), c(0.3, 0.7))
> # Initialize the Markov chain at state 0
> X <- 0 (\( \sigma \)
           X1 - X10000
> for(i in 2:n){
      # Specify row of P for next step probability
+
      row_n <- X[i - 1] + 1
+
                   X[1] H
+
+ # Take next step of Markov chain
      X[i] \leftarrow sample(c(0, 1), size = 1, prob = P[row_n, ])
+
+ }
```

```
> # Proportion of steps in state 0
> sum(X == 0) / n
[1] 0.6013

> # Proportion of steps in state 1
> sum(X == 1) / n
[1] 0.3987
```

What if we started the chain from a different initial state?

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```
> set.seed(999) # for reproduceability
> # Initialize the Markov chain at state 1
> X <- 1
> for(i in 2:n){
      # Specify row of P for next step probability
+
      row_n <- X[i - 1] + 1
+
+
      # Take next step of Markov chain
+
      X[i] \leftarrow sample(c(0, 1), size = 1, prob = P[row_n,])
+
+ }
> sum(X == 0) / n # Proportion of steps in state 0
[1] 0.6061
> sum(X == 1) / n # Proportion of steps in state 1
[1] 0.3939
```

- Let  $\pi_0$  denote the long run (relative) frequency at state 0.
  - From our simulation, we found  $\pi_0 = 0.6$ . (a bob)
- Let  $\pi_1$  denote the long run (relative) frequency at state 1.
  - From our simulation, we found  $\pi_1 = 0.4$ . (0.344)
- Then  $\pi = (\pi_0, \pi_1)$  is a distribution on the state space  $\{0, 1\}$ .
- How do we interpret this distribution?

## Interpretation: (pro and step)

- The fraction of time (steps) in state j is  $\pi_j$ .
  - If n=10000, the number of steps in state 0 is about  $\pi_0 \cdot n = 0.6 \cdot 10000$ . = how time stay  $0 \rightarrow$  4000 stay 1
- ② The probability that  $X_n$  is in state j is  $\pi_j$ . The probability that  $X_n$  is in state j is  $\pi_j$ .
  - $\lim_{n\to\infty} P(X_n=0|X_0=0)=\pi_0=0.6$ (bood time >>)

    —) limiting distribution
  - $\lim_{n \to \infty} P(X_n = 0 | X_0 = 1) = \pi_0 = 0.6$
  - This distribution is independent of the initial state  $X_0$ .

X1 X2 X3 ... Xn lid

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#### Definition

Let  $\pi=(\pi_0,\pi_1,\pi_2,\ldots,\pi_N)$  be a probability distribution on the state space  $\{0,1,2,\ldots,N\}$ . We say  $\pi$  is the **limiting distribution** of a Markov chain  $\{X_0,X_1,X_2,\ldots\}$  if  $f=(x_0,x_1,x_2,\ldots)$  if  $f=(x_0,x_1,x_2,\ldots)$  jewtone

for all  $i, j \in \{0, 1, 2, \dots, N\}$ . P(fine  $i \longrightarrow toj$ ) =  $\pi_j$ 

$$p(from i \longrightarrow t \circ i) = T i$$
  $i \in (0, N)$ 

If the limiting distribution  $\pi = (\pi_0, \pi_1, \pi_2, \dots, \pi_N)$  exists, then  $\pi_j$  represents:

- The probability that  $X_n$  is in state j, independent of the initial state  $X_0$ .
- The long run mean (i.e., expected) fraction of time that the Markov chain  $\{X_t: t=0,1,2,\ldots\}$  spends in state j.

#### Main Questions:

- What conditions will guarantee the existence of the limiting distribution?
- If the limiting distribution exists, how do we find it?

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Question: If the limiting distribution exists, how do we find it?

Suppose we know that the limiting distribution  $\pi$  exists. Then, for n large enough,  $x_0 \longrightarrow x_1 \longrightarrow x$ 

$$P(X_n=k|X_0=i)=\pi_k \text{ and } P(X_{n+1}=j|X_0=i)=\pi_j,$$
 for any  $j,k\in\{0,1,2,\ldots,N\}$ . 
$$0\longrightarrow X_n$$

How can we use these probabilities to solve for

$$\pi = (\pi_0, \pi_1, \pi_2, \dots, \pi_N)$$
?

we total probability

Recall:

#### Law of Total Probability (Discrete)

Let X and Y be discrete random variables. Then

$$P(X=x) = \sum_{y} P(X=x,Y=y)$$

$$= \sum_{y} P(X=x|Y=y)P(Y=y). \text{ (conditional)}$$

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 $\rightarrow \pi(x)$ 

## The Limiting Distribution (long run)

By the Law of Total Probability, we have

$$\pi_{j} = P(X_{n+1} = j | X_{0} = i)$$

$$= \sum_{k=0}^{N} P(X_{n+1} = j, X_{n} = k | X_{0} = i)$$

$$= \sum_{k=0}^{N} P(X_{n+1} = j | X_{n} = k, X_{0} = i) P(X_{n} = k | X_{0} = i)$$

$$\left( \begin{array}{c} \text{Markov} \\ \text{Property} \end{array} \right) = \sum_{k=0}^{N} P_{kj} \pi_{k}$$

$$= \sum_{k=0}^{N} P_{kj} \pi_{k}$$

$$= \sum_{k=0}^{N} \pi_{k} P_{kj},$$

$$\chi_{n-k} | \chi_{n-k} = \chi_{n} | \chi_{n-k} = \chi_{n-k} | \chi_{n-k} | \chi_{n-k} = \chi_{n-k} | \chi_{n-k} | \chi_{n-k} | \chi_{n-k} = \chi_{n-k} | \chi_{n-k} | \chi_{n-k} | \chi_{n-k} | \chi_{n-k}$$

where  $P_{kj} = P(X_{n+1} = j | X_n = k)$  is the one-step transition probability from k to j. Sum (plans state  $\rightarrow$ j)

• We therefore have the relations equations

$$\pi_j = \sum_{k=0}^N \pi_k P_{kj}$$
, for  $j=0,1,2,\ldots,N$ .

• In addition, since  $\pi$  is a probability distribution, then

$$\sum_{i=0}^{N} \pi_i = \pi_0 + \pi_1 + \pi_2 + \cdots + \pi_N = 1.$$
 first equation

- This defines a system of N+2 linear equations for N+1 unknowns (one equation is redundant).
- A solution  $\pi$  to this system of linear equations is called a stationary distribution of the Markov chain.
- In particular, the limiting distribution (if it exists) is a stationary distribution.

   π<sub>1</sub> (π<sub>0</sub> ···· π<sub>1</sub>) → stationary distribution

## **Example 1: Two-State Markov Chain**

• Consider a two-state Markov chain, with state space  $\{0,1\}$ and transition matrix

$$\mathbb{P} = \begin{bmatrix} P_{00} & P_{01} \\ P_{10} & P_{11} \end{bmatrix} = \begin{bmatrix} 0.8 & 0.2 \\ 0.3 & 0.7 \end{bmatrix}.$$

• We want to find a 
$$\pi=(\pi_0,\pi_1)$$
 that satisfies 
$$\pi_0 = \pi_0 P_{00} + \pi_1 P_{10} = p(0.0) \cdot p(0) + p(1.0) \cdot p(1)$$
 which is the satisfies 
$$\pi_1 = \pi_0 P_{00} + \pi_1 P_{10} = p(0.0) \cdot p(0) + p(1.0) \cdot p(1)$$
 and 
$$\pi_0 + \pi_1 = 1.$$

## **Example 1: Two-State Markov Chain**

Plugging in the values from the transition matrix  $\mathbb{P}$ , we have

$$\pi_0 = \pi_0 \cdot 0.8 + \pi_1 \cdot 0.3$$

$$\pi_1 = \pi_0 \cdot 0.2 + \pi_1 \cdot 0.7$$

which simplify to

$$0.2\pi_0 = 0.3\pi_1$$
$$0.3\pi_1 = 0.2\pi_0.$$

Both equations yield the relation

$$\frac{\pi_0}{\pi_1} = \frac{3}{2}.$$

Then, since  $\pi_0 + \pi_1 = 1$ , we have

This corresponds to the limiting distribution we previously found.

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## **Stationary Distributions**

#### Definition

Let  $\{X_0, X_1, X_2, \ldots\}$  be a Markov chain, with state space  $\{0, 1, 2, \ldots, N\}$  and transition matrix  $\mathbb{P} = [P_{ij}]$ . The (row) vector  $\pi = (\pi_0, \pi_1, \pi_2, \ldots, \pi_N)$  is called a **stationary distribution** of the Markov chain if it satisfies:  $\pi = \pi_1$ 

$$\pi_j = \sum_{k=0}^N \pi_k P_{kj}, \quad \text{ for } j = 0, 1, 2, \dots, N,$$

or, equivalently (in matrix notation),  $\pi = \pi \mathbb{P}$ .

$$\sum_{i=0}^{N} \pi_i = 1$$
. first equation

## **Example 2: Identity Transition Matrix**



Consider a two-state Markov chain with transition matrix

$$\mathbb{P} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = I_2. \qquad \begin{bmatrix} \pi_{\bullet} \\ \pi_{\bullet} \end{bmatrix} \begin{bmatrix} 0 \\ \pi_{\bullet} \end{bmatrix} = \begin{bmatrix} \tilde{\pi}_{\bullet} \\ \pi_{\bullet} \end{bmatrix}$$

- Notice that  $\pi I_2 = \pi$  for every vector  $\pi$ .
- Therefore, there are infinitely many stationary distributions for this Markov chain.
- In particular, stationary distributions may not be unique.

many solution

One solution

PNE

## Example 3: Two-State Markov Chain (Revisited)

• Consider a two-state Markov chain, with state space  $\{0,1\}$  and transition matrix

$$\mathbb{P} = \begin{bmatrix} 0.8 & 0.2 \\ 0.3 & 0.7 \end{bmatrix}.$$

- Let  $\pi = (\pi_0, \pi_1) = (0.6, 0.4)$  denote a stationary distribution for this Markov chain.
- Suppose  $X_0 \sim \pi$ . We want to show that  $X_1 \sim \pi$ .

## Example 3: Two-State Markov Chain (Revisited)

If 
$$P(X_0 = 0) = \pi_0 = 0.6$$
 and  $P(X_0 = 1) = \pi_1 = 0.4$ , then 
$$P(X_1 = 0) = \sum_{i=0}^{1} P(X_1 = 0, X_0 = i)$$

$$= P(X_1 = 0, X_0 = 0) + P(X_1 = 0, X_0 = 1)$$

$$= P(X_1 = 0 | X_0 = 0) P(X_0 = 0)$$

$$= P(X_1 = 0 | X_0 = 0) P(X_0 = 0)$$

$$+ P(X_1 = 0 | X_0 = 1) P(X_0 = 1)$$

$$= P(X_1 = 0 | X_0 = 1) P(X_0 = 1)$$

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$$= P(X_1 = 0 | X_0 = 1) P(X_0 = 1)$$

$$= P(X_1 = 0 | X_$$

$$P(X_1 = 1) = 1 - 0.6 = 0.4 = \pi_1.$$

So  $X_1 \sim \pi_1$ .

## **Stationary Distributions**

- Let  $\pi$  be a stationary distribution of a Markov chain. If  $X_0 \sim \pi$ , then  $X_1 \sim \pi$ . This implies that  $X_n \sim \pi$  for every n.
- In other words, if the initial distribution for  $X_0$  is a stationary distribution  $\pi$ , then  $\pi$  is the common distribution for all  $X_n$  in the Markov chain (and we say the Markov chain is **stationary**).

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## Example 4: Two-State Markov Chain (General)

• Consider a two-state Markov chain, with state space  $\{0,1\}$  and transition matrix

$$\mathbb{P} = \begin{bmatrix} 1 - a & a \\ b & 1 - b \end{bmatrix},$$

for some a, b > 0.

• We want to find a stationary distribution  $\pi = (\pi_0, \pi_1)$ .

## Example 4: Two-State Markov Chain (General)

For  $\pi = (\pi_0, \pi_1)$  to be a stationary distribution, it must satisfy

$$\pi = \pi \mathbb{P}$$

$$[\pi_0 \quad \pi_1] = [\pi_0 \quad \pi_1] \begin{bmatrix} 1 - a & a \\ b & 1 - b \end{bmatrix} \rightarrow \text{stay}$$

$$= [(1 - a)\pi_0 + b\pi_1 \quad a\pi_0 + (1 - b)\pi_1],$$
equates to

which equates to 

$$\pi_1 = a\pi_0 + (1-b)\pi_1.$$
 Solve

These equations give the relation  $a\pi_0 = b\pi_1$ , or

$$\frac{\pi_0}{\pi_1} = \frac{b}{a} \cdot \frac{o.b}{o.\psi} = \frac{5}{2}$$

Then, since  $\pi_0 + \pi_1 = 1$ , we have

$$\pi_0 = rac{b}{a+b}$$
 and  $\pi_1 = rac{a}{a+b}$ .

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## Conditions for the Limiting Distribution

#### Conditions for the Limiting Distribution

Let  $\{X_0, X_1, X_2, \ldots\}$  be a Markov chain with state space  $\{0, 1, 2, \ldots, N\}$  and transition matrix  $\mathbb{P}$ . The Markov chain has a limiting distribution if:

There is a solution to the system of equations defined by

$$\begin{cases} \pi = \pi \mathbb{P} \\ \sum_{i=0}^{N} \pi_i = 1 \end{cases}$$

i.e., there is a stationary distribution. (1) get solution

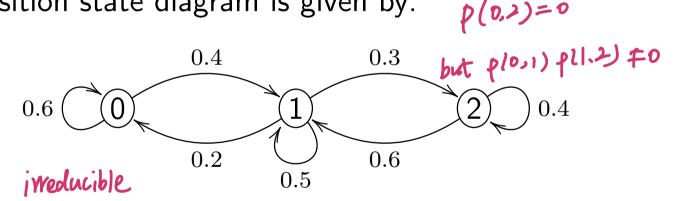
- 2 The Markov chain is irreducible. 5 states communicate
- The Markov chain is aperiodic. (3) period=1

#### Irreducible Markov Chains

• Consider a three-state Markov chain, with state space  $\{0,1,2\}$  and transition matrix

$$\mathbb{P} = \begin{bmatrix} 0.6 & 0.4 & 0 \\ 0.2 & 0.5 & 0.3 \\ 0 & 0.6 & 0.4 \end{bmatrix}.$$

• A transition state diagram is given by: p(0,2)=



• Notice that state 0 cannot jump to state 2 directly  $(P_{02} = 0)$ , but (by following the arrows on the diagram) there is a path from state 0 to state 2:  $0 \to 1 \to 2$ .

#### Irreducible Markov Chains

#### Definition

State j is **accessible** from state i, denoted by  $i \rightarrow j$ , if there is a path from state i to state j. P(i j)  $\neq 0$ 

#### Definition

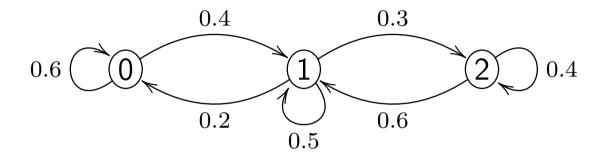
Two states i and j communicate, denoted by  $i \leftrightarrow j$ , if each state is accessible from the other. In other words, if  $i \to j$  and  $j \to i$ , then  $i \leftrightarrow j$ .

#### Definition

A Markov chain is **irreducible** if all states communicate with each other. A Markov chain is **reducible** if it is not irreducible.

## Example 5: An Irreducible Markov Chain

• Consider a Markov chain with transition state diagram:

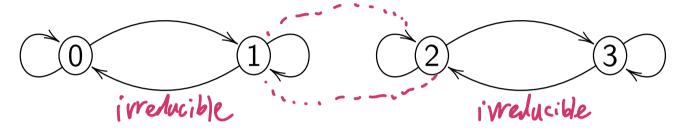


- There is a looped path  $0 \to 1 \to 2 \to 1 \to 0$  which passes through every state in the state space and shows that every state is accessible from any other state.
- Since all states communicate with each other, then this Markov chain is irreducible.

## Example 6: A Reducible Markov Chain

$$\begin{array}{ccc} | \xrightarrow{\times} \rangle 2 & 2 \xrightarrow{\times} | \\ | \xrightarrow{\times} \rangle 3 & 2 \xrightarrow{\times} \rangle 0 \end{array}$$

Consider a Markov chain with transition state diagram:



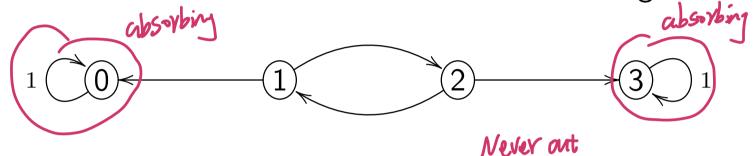
- Notice that 0 

  → 2: There is no path from state 0 to state 2 (or vice versa), so 0 and 2 do not communicate.
- Not all states communicate with each other, so this Markov chain is reducible.

• This Markov chain can be reduced to two Markov chains, each with two states.

## **Example 7: Absorbing States**

• Consider a Markov chain with transition state diagram:



- Notice that states 0 and 3 are <u>absorbing states</u>: Once the Markov chain enters an absorbing state, it never leaves.
- Not all states communicate with each other (e.g.,  $2 \rightarrow 0$  but  $0 \not\rightarrow 2$ , so  $0 \not\leftrightarrow 2$ ), so this Markov chain is reducible.

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## **Example 8: Block Transition Matrix**

• Consider a Markov chain with state space  $\{0,1,2,3,4\}$  and transition matrix:

$$\mathbb{P} = \begin{bmatrix} 1/2 & 1/2 & 0 & 0 & 0 \\ 1/4 & 3/4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1/2 & 0 & 1/2 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}.$$

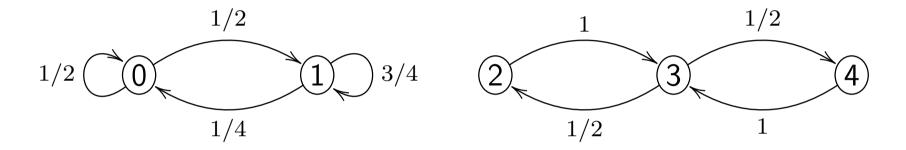
Is this Markov chain irreducible or reducible?

reducible

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## **Example 8: Block Transition Matrix**

• A transition state diagram for this transition matrix is given by:



- We see that  $0 \leftrightarrow 1$ ,  $2 \leftrightarrow 3$ ,  $3 \leftrightarrow 4$ , and  $2 \leftrightarrow 4$ , but  $\{0,1\} \not\leftrightarrow \{2,3,4\}$ .
- Not all states communicate with each other, so this Markov chain is reducible.

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## **Example 8: Block Transition Matrix**

• Notice that  $\mathbb{P}$  is a block diagonal transition matrix:

$$\mathbb{P} = \begin{bmatrix} 1/2 & 1/2 & 0 & 0 & 0 \\ 1/4 & 3/4 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1/2 & 0 & 1/2 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

• The blocks of zeroes on the block off-diagonals indicate that states within each block are not accessible from states in other blocks.

#### Irreducible Markov Chains

Accessibility can be defined more rigorously using n-step transition probabilities:

#### Definition

Let  $\{X_0, X_1, X_2, \ldots\}$  be a Markov chain with state space  $\{0, 1, 2, \ldots, N\}$ . The n-step transition probability from state i to j is defined by

$$P_{ij}^{(n)} := P(X_n = j | X_0 = i).$$

Note that when n=1,  $P_{ij}^{(1)}=P_{ij}$ .

#### Definition

State j is **accessible** from state i, denoted by  $i \to j$ , if there is positive probability that state j can be reached from state i in a finite number of transitions. In other words,  $P_{ij}^{(n)} > 0$  for some n.

## Periodicity of a Markov Chain

#### Definition

The **period** of a state i, denoted by d(i), is the greatest common divisor (gcd) of all integers  $n \ge 1$  for which  $P_{ii}^{(n)} > 0$ .

To find the period of a state i, we consider the number of steps it takes for any path starting from state i to return to state i.

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## **Example 9: Absorbing States (Revisited)**

• Consider a Markov chain with state space  $\{0,1,2,3\}$  and transition matrix

$$\mathbb{P} = \frac{1}{2} \begin{bmatrix} 1 & 0 & 0 & 0 \\ q & 0 & p & 0 \\ 0 & q & 0 & p \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad 0$$

where 0 < p, q < 1.

reducible

• We want to find the period d(i) of each state  $i \in \{0, 1, 2, 3\}$ .

$$| d(1) = | \rightarrow 2 \rightarrow 1 = 2$$

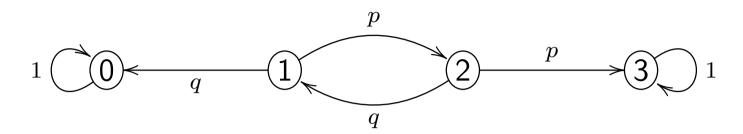
$$2 d(2) : 2 \rightarrow 1 \rightarrow 2 = 2$$

$$3 d(3) = |$$

$$0 d(4) = |$$

## **Example 9: Absorbing States (Revisited)**

A transition state diagram for this transition matrix is given by:



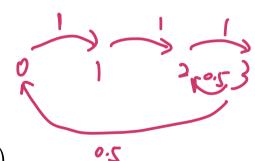
- d(0): d(0) = 1, because  $P_{00} > 0$ .
- d(1): There is a path  $1 \rightarrow 2 \rightarrow 1$ , so  $P_{11}^{(2)} > 0$ .
  - There is a path  $1 \to 2 \to 1 \to 2 \to 1$ , so  $P_{\text{11}}^{(4)} > 0$ .
  - All number of steps n such that  $P_{11}^{(n)} > 0$ :  $\{2, 4, \underline{6}, \underline{8, ...} \}$ .
  - $gcd\{2,4,6,8,\ldots\} = 2$ , so d(1) = 2.
- d(2): States 1 and 2 are symmetric, so d(2) = 2.
- d(3): d(3) = 1, because  $P_{33} > 0$ .

-> not aperiodic

## Example 10: One Big Loop

ullet Consider a Markov chain with state space  $\{0,1,2,3\}$  and transition matrix

$$\mathbb{P} = \begin{bmatrix} 0 & (1) & 0 & 0 \\ 0 & (1) & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1/2 & 0 & 1/2 & 0 \end{bmatrix}.$$



• We want to find the period of state 0: d(0).

$$0 \rightarrow 1 \rightarrow 2 \rightarrow 3 \rightarrow 0 = 4$$

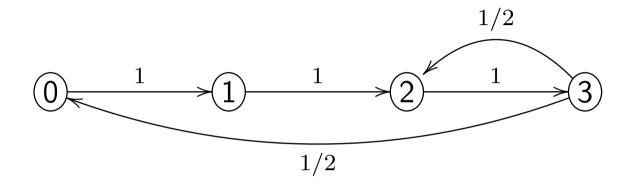
$$0 \rightarrow 1 \rightarrow 2 \rightarrow 3 \rightarrow 2 \rightarrow 3 \rightarrow 0 = 6$$

$$9 cd: \{4, 6, 8, 10 \cdots \}$$

$$d(a) = 2$$

## Example 10: One Big Loop

A transition state diagram for this transition matrix is given by:



- There is a path  $0 \to 1 \to 2 \to 3 \to 0$ , so  $P_{00}^{(4)} > 0$ .
- There is a path  $0 \to 1 \to 2 \to 3 \to 2 \to 3 \to 0$ , so  $P_{00}^{(6)} > 0$ .
- All numbers of steps n such that  $P_{00}^{(n)} > 0$ :  $\{4, 6, 8, 10, \ldots\}$ .
- $gcd{4,6,8,10,...} = 2$ , so d(0) = 2.

## Periodicity of a Markov Chain

#### Definition

A Markov chain is called aperiodic if each state has period 1.)

Some ways to check if a Markov chain is aperiodic:

- If  $P_{ii} > 0$ , then d(i) = 1.
- If  $i \leftrightarrow j$  and  $P_{ii} > 0$ , then d(j) = 1.  $\rightarrow$

 $i \rightarrow i+1 \rightarrow i+2 \rightarrow j$ 

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## Periodicity of a Markov Chain

**Show**: If  $i \leftrightarrow j$  and  $P_{ii} > 0$ , then d(j) = 1.

- Since  $i \leftrightarrow j$ , then there is a k-step path from  $j \to i$ , denoted by  $j \overset{k}{\leadsto} i$ , and an m-step path from  $i \to j$ , denoted by  $i \overset{m}{\leadsto} j$ , for some k, m. Then  $j \overset{k}{\leadsto} i \overset{m}{\leadsto} j$  is a (k+m)-step path from j to j. So  $P_{jj}^{(k+m)} > 0$ .
- Since i has a self-loop  $(P_{ii} > 0)$ , then  $j \stackrel{k}{\leadsto} i \rightarrow i \stackrel{m}{\leadsto} j$  is a (k+m+1)-step path from j to j, so  $P_{jj}^{(k+m+1)} > 0$ .
- gcd(k+m, k+m+1) = 1, so d(j) = 1.

## The Basic Limit Theorem of Markov Chains

#### The Basic Limit Theorem of Markov Chains

If a Markov chain  $\{X_0, X_1, X_2, \ldots\}$  is irreducible, aperiodic, and has a stationary distribution  $\pi = (\pi_0, \pi_1, \pi_2, \ldots, \pi_N)$ , then

$$\lim_{n\to\infty} P(X_n = j|X_0 = i) = \pi_j.$$

That is,  $\pi$  is the limiting distribution of the Markov chain, and  $\pi$  is uniquely determined by the system of equations

$$\begin{cases} \pi = \pi \mathbb{P} \\ \sum_{i=0}^{N} \pi_i = 1 \end{cases}$$

where  $\mathbb{P}$  is the transition matrix of the Markov chain.

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