STAT253/317 Lecture 3: Two key questions

1. As time goes to infinity, does the fraction of time spent in a given state converge? Mathematically, we aim to study

$$\lim_{n\to\infty} \frac{\sum_{i=0}^{n-1} 1\{X_i = k\}}{n}.$$

2. As time goes to infinity, does the probability of being in a given state converge to a limit? This is given by

$$\lim_{n\to\infty} P_{ij}^{(n)}.$$

Stationary Distribution

Define $\pi_i^{(n)} = \mathrm{P}(X_n = i)$, $i \in \mathfrak{X}$ to be the marginal distribution of X_n, $n = 1, 2, \ldots$, and let $\pi^{(n)}$ be the row vector

$$\pi^{(n)} = (\pi_0^{(n)}, \pi_1^{(n)}, \pi_2^{(n)}, \ldots),$$

From Chapman-Kolmogrov Equation, we know that

$$\pi^{(n)} = \pi^{(n-1)}\mathbb{P} \quad \text{i.e.} \quad \pi_j^{(n)} = \sum\nolimits_{i\in\mathfrak{X}} \pi_i^{(n-1)} P_{ij} \text{ for all } j \in \mathfrak{X},$$

If π is a distribution on $\mathfrak{X}$ satisfying

$$\pi\mathbb{P} = \pi \quad \text{i.e.} \quad \pi_j = \sum\nolimits_{i\in\mathfrak{X}} \pi_i P_{ij} \text{ for all } j \in \mathfrak{X},$$

then $\pi^{(0)} = \pi$ implies $\pi^{(n)} = \pi$ for all n.

We say π is a **stationary distribution** of the Markov chain.

Example 1: 2-state Markov Chain

$$\mathfrak{X} = \{0, 1\}, \qquad \mathbb{P} = \begin{array}{c c} & \begin{array}{cc} 0 & 1 \end{array} \\ \begin{array}{c} 0 \\ 1 \end{array} & \begin{pmatrix} 1-\alpha & \alpha \\ \beta & 1-\beta \end{pmatrix} \end{array}$$

$$\pi\mathbb{P} = \pi \Rightarrow \begin{cases} \pi_0 & = (1-\alpha)\pi_0 + \beta\pi_1 \\ \pi_1 & = \alpha\pi_0 + (1-\beta)\pi_1 \end{cases}$$

$$\Rightarrow \begin{cases} \alpha\pi_0 & = \beta\pi_1 \\ \beta\pi_1 & = \alpha\pi_0 \end{cases}$$

Need one more constraint: $\pi_0 + \pi_1 = 1$

$$\Rightarrow \pi = (\pi_0, \pi_1) = \left(\frac{\beta}{\alpha+\beta}, \frac{\alpha}{\alpha+\beta}\right)$$

Example 2: Ehrenfest Diffusion Model with N Balls

$$P_{ij} = \begin{cases} \dfrac{i}{N} & \text{if } j = i-1 \\ \dfrac{N-i}{N} & \text{if } j = i+1 \\ 0 & \text{otherwise} \end{cases}$$

$$\begin{aligned}
\pi_0 &= \pi_1 P_{10} = \tfrac{1}{N}\pi_1 \Rightarrow \pi_1 = N\pi_0 = \tbinom{N}{1}\pi_0 \\
\pi_1 &= \pi_0 P_{01} + \pi_2 P_{21} = \pi_0 + \tfrac{2}{N}\pi_2 \Rightarrow \pi_2 = \tfrac{N(N-1)}{2}\pi_0 = \tbinom{N}{2}\pi_0 \\
\pi_2 &= \pi_1 P_{12} + \pi_3 P_{32} = \tfrac{N-1}{N}\pi_1 + \tfrac{3}{N}\pi_3 \Rightarrow \pi_3 = \tfrac{N(N-1)(N-2)}{6}\pi_0 = \tbinom{N}{3}\pi_0 \\
&\vdots \qquad\qquad \vdots
\end{aligned}$$

In general, you'll get $\pi_i = \binom{N}{i}\pi_0$.
As $1 = \sum_{i=0}^{N} \pi_i = \pi_0 \sum_{i=0}^{N} \binom{N}{i}$ and $\sum_{i=0}^{N} \binom{N}{i} = 2^N$, we have

$$\pi_i = \binom{N}{i}\left(\frac{1}{2}\right)^N \quad \text{for } i = 0, 1, 2, \ldots, N.$$

Stationary Distribution May Not Be Unique

Consider a Markov chain with transition matrix $\mathbb{P}$ of the form

$$\mathbb{P} = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \!\!\begin{array}{c} \begin{array}{ccccc} 0 & 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} * & * & 0 & 0 & 0 \\ * & * & 0 & 0 & 0 \\ 0 & 0 & * & * & * \\ 0 & 0 & * & * & * \\ 0 & 0 & * & * & * \end{pmatrix} \end{array} = \begin{pmatrix} \mathbb{P}_x & 0 \\ 0 & \mathbb{P}_y \end{pmatrix}$$

This Markov chain has 2 classes {0,1} and {2, 3, 4}; both are recurrent. Note that this Markov chain can be reduced to two sub-Markov chains, one with state space {0,1} and the other {2, 3, 4}. Their transition matrices are respectively $\mathbb{P}_x$ and $\mathbb{P}_y$.

Say $\pi_x = (\pi_0, \pi_1)$ and $\pi_y = (\pi_2, \pi_3, \pi_4)$ be respectively the stationary distributions of the two sub-Markov chains, i.e.,

$$\pi_x \mathbb{P}_x = \pi_x, \quad \pi_y \mathbb{P}_y = \pi_y$$

Verify that $\pi = (c\pi_0, c\pi_1, (1-c)\pi_2, (1-c)\pi_3, (1-c)\pi_4)$ is a stationary distribution of $\{X_n\}$ for any c between 0 and 1.

Not All Markov Chains Have a Stationary Distribution

For one-dimensional symmetric random walk, the transition probabilities are

$$P_{i,i+1} = P_{i,i-1} = 1/2$$

The stationary distribution $\{\pi_j\}$ would satisfy the equation:

$$\pi_j = \sum_{i \in \mathfrak{X}} \pi_i P_{ij} = \frac{1}{2}\pi_{j-1} + \frac{1}{2}\pi_{j+1}.$$

Once π_0 and π_1 are determined, all π_j's can be determined from the equations as

$$\pi_j = \pi_0 + (\pi_1 - \pi_0)j, \quad \text{for all integer } j.$$

As $\pi_j \geq 0$ for all integer j, $\Rightarrow \pi_1 = \pi_0$. Thus

$$\pi_j = \pi_0 \quad \text{for all integer } j$$

Impossible to make $\sum_{j=-\infty}^{\infty} \pi_j = 1$.

Conclusion: 1-dim symmetric random walk does not have a stationary distribution.

Limiting Distribution

A probability distribution $\pi = [\pi_0, \pi_1, \pi_2, \dots]$ is called the limiting distribution of a Markov chain X_n if for all $i, j \in \mathfrak{X}$,

$$\pi_j = \lim_{n\to\infty} P_{ij}^{(n)} = \lim_{n\to\infty} \mathrm{P}(X_n = j \mid X_0 = i)$$

Matrix version

$$\text{i.e.,} \quad \lim_{n\to\infty} \mathbb{P}^{(n)} = \begin{pmatrix} \pi_0 & \pi_1 & \pi_2 & \pi_3 & \cdots \\ \pi_0 & \pi_1 & \pi_2 & \pi_3 & \cdots \\ \pi_0 & \pi_1 & \pi_2 & \pi_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Example: Two-State Markov Chain

$$\mathfrak{X} = \{0, 1\}, \qquad \mathbb{P} = \begin{array}{c c} & \begin{array}{cc} 0 & \quad 1 \end{array} \\ \begin{array}{c} 0 \\ 1 \end{array} & \begin{pmatrix} 1-\alpha & \alpha \\ \beta & 1-\beta \end{pmatrix} \end{array}$$

By induction, one can show that

$$\mathbb{P}^{(n)} = \begin{pmatrix} \dfrac{\beta}{\alpha+\beta} + \dfrac{\alpha}{\alpha+\beta}(1-\alpha-\beta)^n & \dfrac{\alpha}{\alpha+\beta} - \dfrac{\alpha}{\alpha+\beta}(1-\alpha-\beta)^n \\ \dfrac{\beta}{\alpha+\beta} + \dfrac{\beta}{\alpha+\beta}(1-\alpha-\beta)^n & \dfrac{\alpha}{\alpha+\beta} - \dfrac{\beta}{\alpha+\beta}(1-\alpha-\beta)^n \end{pmatrix}$$

$$\to \begin{pmatrix} \dfrac{\beta}{\alpha+\beta} & \dfrac{\alpha}{\alpha+\beta} \\ \dfrac{\beta}{\alpha+\beta} & \dfrac{\alpha}{\alpha+\beta} \end{pmatrix} \quad \text{as } n \to \infty$$

The limiting distribution π is $(\frac{\beta}{\alpha+\beta}, \frac{\alpha}{\alpha+\beta})$.

Limiting Distribution is a Stationary Distribution

The limiting distribution of a Markov chain is a stationary distribution of the Markov chain.

Proof *(not rigorous).* By Chapman Kolmogorov Equation,

$$P_{ij}^{(n+1)} = \sum_{k \in \mathfrak{X}} P_{ik}^{(n)} P_{kj}$$

Letting $n \to \infty$, we get

$$\begin{aligned} \pi_j = \lim_{n\to\infty} P_{ij}^{(n+1)} &= \lim_{n\to\infty} \sum_{k \in \mathfrak{X}} P_{ik}^{(n)} P_{kj} \\ &=^* \sum_{k \in \mathfrak{X}} \lim_{n\to\infty} P_{ik}^{(n)} P_{kj} \quad \text{(needs justification)} \\ &= \sum_{k \in \mathfrak{X}} \pi_k P_{kj} \end{aligned}$$

Thus the limiting distribution π_j's satisfies the equations $\pi_j = \sum_{k \in \mathfrak{X}} \pi_k P_{kj}$ for all $j \in \mathfrak{X}$ and is a stationary distribution.

See Karlin & Taylor (1975), Theorem 1.3 on p.85-86 for a rigorous proof.

Not All Markov Chains Have Limiting Distributions

Consider the simple random walk X_n on $\{0, 1, 2, 3, 4\}$ with absorbing boundary at 0 and 4. That is,

$$X_{n+1} = \begin{cases} X_n + 1 & \text{with probability 0.5 if } 0 < X_n < 4 \\ X_n - 1 & \text{with probability 0.5 if } 0 < X_n < 4 \\ X_n & \text{if } X_n = 0 \text{ or } 4 \end{cases}$$

The transition matrix is hence

$$\mathbb{P} = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{ccccc} 0 & 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0.5 & 0 & 0.5 & 0 & 0 \\ 0 & 0.5 & 0 & 0.5 & 0 \\ 0 & 0 & 0.5 & 0 & 0.5 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \end{array}$$

Not All Markov Chains Have Limiting Distributions

The n-step transition matrix of the simple random walk X_n on $\{0, 1, 2, 3, 4\}$ with absorbing boundary at 0 and 4 can by shown by induction using the Chapman-Kolmogorov Equation to be

$$\mathbb{P}^{(2n-1)} = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{ccccc} 0 & 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0.75 - 0.5^{n+1} & 0 & 0.5^n & 0 & 0.25 - 0.5^{n+1} \\ 0.5 - 0.5^n & 0.5^n & 0 & 0.5^n & 0.5 - 0.5^n \\ 0.25 - 0.5^{n+1} & 0 & 0.5^n & 0 & 0.75 - 0.5^{n+1} \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \end{array}$$

$$\mathbb{P}^{(2n)} = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{ccccc} 0 & 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0.75 - 0.5^{n+1} & 0.5^{n+1} & 0 & 0.5^{n+1} & 0.25 - 0.5^{n+1} \\ 0.5 - 0.5^{n+1} & 0 & 0.5^n & 0 & 0.5 - 0.5^{n+1} \\ 0.25 - 0.5^{n+1} & 0.5^{n+1} & 0 & 0.5^{n+1} & 0.75 - 0.5^{n+1} \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \end{array}$$

Not All Markov Chains Have Limiting Distributions

The limit of the n-step transition matrix as $n \to \infty$ is

$$\mathbb{P}^{(n)} \to \begin{array}{c c} & \begin{array}{ccccc} 0 & 1 & 2 & 3 & 4 \end{array} \\ \begin{array}{c} 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{array} & \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0.75 & 0 & 0 & 0 & 0.25 \\ 0.5 & 0 & 0 & 0 & 0.5 \\ 0.25 & 0 & 0 & 0 & 0.75 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \end{array}.$$

Though $\lim_{n\to\infty} P_{ij}^{(n)}$ exists but the limit depends on the initial state i, this Markov chain has no limiting distribution.

This Markov chain has two distinct absorbing states 0 and 4. Other transient states may be absorbed to either 0 or 4 with different probabilities depending how close those states are to 0 or 4.

When does a Markov chain have limiting distribution?

Periodicity

A state of a Markov chain is said to have **period** d if

$$P_{ii}^{(n)} = 0, \quad \text{whenever } n \text{ is not a multiple of } d$$

In other words, d is the *greatest common divisor* of all the n's such that

$$P_{ii}^{(n)} > 0$$

We say a state is **aperiodic** if $d = 1$, and **periodic** if $d > 1$.

Fact: Periodicity is a class property.
That is, all states in the same class have the same period.

For a proof, see Problem 2&3 on p.77 of Karlin & Taylor (1975).

Examples (Periodicity)

- All states in the Ehrenfest diffusion model are of period $d = 2$ since it's impossible to move back to the initial state in odd number of steps.
- 1-D (2-D) Simple random walk on all integers (grids on a 2-d plane) are of period $d = 2$

Example (Periodicity)

Specify the classes of a Markov chain with the following transition matrix, and find the periodicity for each state.

$$
\begin{array}{cc}
 & \begin{array}{ccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 \end{array} \\
\begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \end{array} &
\begin{pmatrix}
0 & 0.5 & 0 & 0.5 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0.5 & 0 & 0 & 0 & 0 & 0.5 & 0 \\
0 & 0 & 0.5 & 0 & 0.5 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0.1 & 0.9 \\
0 & 0 & 0 & 0 & 0 & 0.7 & 0.3
\end{pmatrix}
\end{array}
$$

$$
\begin{array}{ccccc}
5 & \rightarrow & 1 & \rightarrow & 2 \\
\uparrow & \swarrow & \uparrow & \swarrow & \\
4 & \rightarrow & 3 & & \\
 & & \downarrow & & \\
7 & \leftrightarrow & 6 & &
\end{array}
$$

Classes: $\{1,2,3,4,5\}$, $\{6,7\}$.
Period is $d = 1$ for state 6 and 7.
Period is $d = 3$ for state 1,2,3,4,5 since
$\{1\} \rightarrow \{2,4\} \rightarrow \{3,5\} \rightarrow \{1\}$.

Periodic Markov Chains Have No Limiting Distributions

For example, in the Ehrenfest diffusion model with 4 balls, it can be shown by induction that the $(2n-1)$-step transition matrix is

$$\mathbb{P}^{(2n-1)} = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{ccccc} 0 & 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} 0 & 1/2+1/2^{2n-1} & 0 & 1/2-1/2^{2n-1} & 0 \\ 1/8+1/2^{2n+1} & 0 & 3/4 & 0 & 1/8-1/2^{2n+1} \\ 0 & 1/2 & 0 & 1/2 & 0 \\ 1/8-1/2^{2n+1} & 0 & 3/4 & 0 & 1/8+1/2^{2n+1} \\ 0 & 1/2-1/2^{2n-1} & 0 & 1/2+1/2^{2n-1} & 0 \end{pmatrix} \end{array}$$

$$\to \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{ccccc} 0 & 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} 0 & 1/2 & 0 & 1/2 & 0 \\ 1/8 & 0 & 3/4 & 0 & 1/8 \\ 0 & 1/2 & 0 & 1/2 & 0 \\ 1/8 & 0 & 3/4 & 0 & 1/8 \\ 0 & 1/2 & 0 & 1/2 & 0 \end{pmatrix} \end{array} \quad \text{as } n \to \infty.$$

Periodic Markov Chains Have No Limiting Distributions

and the $2n$-step transition matrix is

$$\mathbb{P}^{(2n)} = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{ccccc} 0 & 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} 1/8+1/2^{2n+1} & 0 & 3/4 & 0 & 1/8-1/2^{2n+1} \\ 0 & 1/2+1/2^{2n+1} & 0 & 1/2-1/2^{2n+1} & 0 \\ 1/8 & 0 & 3/4 & 0 & 1/8 \\ 0 & 1/2-1/2^{2n+1} & 0 & 1/2+1/2^{2n+1} & 0 \\ 1/8-1/2^{2n+1} & 0 & 3/4 & 0 & 1/8+1/2^{2n+1} \end{pmatrix} \end{array}$$

$$\to \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{ccccc} 0 & 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} 1/8 & 0 & 3/4 & 0 & 1/8 \\ 0 & 1/2 & 0 & 1/2 & 0 \\ 1/8 & 0 & 3/4 & 0 & 1/8 \\ 0 & 1/2 & 0 & 1/2 & 0 \\ 1/8 & 0 & 3/4 & 0 & 1/8 \end{pmatrix} \end{array} \quad \text{as } n \to \infty.$$

Periodic Markov Chains Have No Limiting Distributions

In general for Ehrenfest diffusion model with N balls, as $n \to \infty$,

$$P_{ij}^{(2n)} \to \begin{cases} 2\binom{N}{j}\left(\frac{1}{2}\right)^N & \text{if } i+j \text{ is even} \\ 0 & \text{if } i+j \text{ is odd} \end{cases}$$

$$P_{ij}^{(2n+1)} \to \begin{cases} 0 & \text{if } i+j \text{ is even} \\ 2\binom{N}{j}\left(\frac{1}{2}\right)^N & \text{if } i+j \text{ is odd} \end{cases}$$

$\lim_{n\to\infty} P_{ij}^{(n)}$ doesn't exist for all $i, j \in \mathfrak{X}$

Summary

- Stationary distribution may not be unique if the Markov chain is not irreducible
- Stationary distribution may not exist
- A limiting distribution is always a stationary distribution
- If it exists, limiting distribution is unique
- Limiting distribution do not exist if the Markov chain is periodic