STAT253/317 Winter 2020 Lecture 2

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4.2 Chapman-Kolmogorov Equation

Joint Distribution of Random Variables in a Markov Chain

Suppose $\{X_n : \ n = 0, 1, 2, \ldots\}$ is a stationary Markov chain with

- state space $\mathfrak{X}$ and
- transition probabilities $\{P_{ij} : i, j \in \mathfrak{X}\}$.

Define $\pi_0(i) = \mathrm{P}(X_0 = i)$, $i \in \mathfrak{X}$ to be the distribution of X_0.

What is the joint distribution of X_0, X_1, X_2?

$$
\begin{aligned}
&\mathrm{P}(X_0 = i_0, X_1 = i_1, X_2 = i_2) \\
&= \mathrm{P}(X_0 = i_0)\mathrm{P}(X_1 = i_1 | X_0 = i_0)\mathrm{P}(X_2 = i_2 | X_1 = i_1, X_0 = i_0) \\
&= \mathrm{P}(X_0 = i_0)\mathrm{P}(X_1 = i_1 | X_0 = i_0)\mathrm{P}(X_2 = i_2 | X_1 = i_1) \quad (\because \text{ Markov}) \\
&= \pi_0(i_0) P_{i_0 i_1} P_{i_1 i_2}
\end{aligned}
$$

In general,

$$
\begin{aligned}
&\mathrm{P}(X_0 = i_0, X_1 = i_1, X_2 = i_2, \ldots, X_{n-1} = i_{n-1}, X_n = i_n) \\
&= \pi_0(i_0) P_{i_0 i_1} P_{i_1 i_2} \ldots P_{i_{n-1} i_n}
\end{aligned}
$$

n-Step Transition Probabilities

Suppose $\{X_n\}$ is a stationary Markov chain with state space $\mathfrak{X}$.
Define the n-step transition probabilities

$$P_{ij}^{(n)} = \mathrm{P}(X_{n+k} = j | X_k = i) \quad \text{for } i, j \in \mathfrak{X} \text{ and } n, k = 0, 1, 2, \ldots$$

How to calculate $P_{ij}^{(n)}$?

Example: Ehrenfest Model, 4 Balls

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

Q1 Find $P_{4,2}^{(2)} = \mathrm{P}(X_2 = 2 | X_0 = 4)$.
Only one possible path: $4 \to 3 \to 2$,
so $P_{4,2}^{(2)} = P_{4,3} P_{3,2} = 1 \cdot (3/4) = 3/4$.

Q2 Find $P_{4,2}^{(3)} = \mathrm{P}(X_3 = 2 | X_0 = 4)$.
Impossible to go from 4 to 2 in odd number of steps,
so $P_{4,2}^{(3)} = 0$.

$$\mathbb{P} = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{ccccc} 0 & 1 & 2 & 3 & 4 \end{array} \\ \left(\begin{array}{ccccc} 0 & 1 & 0 & 0 & 0 \\ 1/4 & 0 & 3/4 & 0 & 0 \\ 0 & 2/4 & 0 & 2/4 & 0 \\ 0 & 0 & 3/4 & 0 & 1/4 \\ 0 & 0 & 0 & 1 & 0 \end{array} \right) \end{array}$$

Q3 Find $P^{(4)}_{4,2} = \mathrm{P}(X_4 = 2 | X_0 = 4)$.

Possible paths:

$$\begin{array}{ccccccccc} 4 & \to & 3 & \to & 4 & \to & 3 & \to & 2 \\ & & & \searrow & & \nearrow & & \nearrow & \\ & & & & 2 & \to & 1 & & \end{array}$$

$$\begin{aligned} P^{(4)}_{4,2} &= P_{4,3}P_{3,4}P_{4,3}P_{3,2} + P_{4,3}P_{3,2}P_{2,3}P_{3,2} + P_{4,3}P_{3,2}P_{2,1}P_{1,2} \\ &= 1 \cdot \frac{1}{4} \cdot 1 \cdot \frac{3}{4} + 1 \cdot \frac{3}{4} \cdot \frac{2}{4} \cdot \frac{3}{4} + 1 \cdot \frac{3}{4} \cdot \frac{2}{4} \cdot \frac{3}{4} = \frac{3}{4} \end{aligned}$$

Q4 Find $P^{(10)}_{4,2} = \mathrm{P}(X_{10} = 2 | X_0 = 4)$.

Too many paths to list, likely to miss a few.

Chapman-Kolmogorov Equation

Suppose $\{X_n\}$ is a stationary Markov chain with state space $\mathfrak{X}$.
Define the n-step transition probabilities

$$P_{ij}^{(n)} = \mathrm{P}(X_{n+k} = j | X_k = i) \quad \text{for } i, j \in \mathfrak{X} \text{ and } n, k = 0, 1, 2, \ldots$$

Then for all m, $n \geq 1$,

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

Proof.

$$\begin{aligned}
P_{ij}^{(m+n)} &= \mathrm{P}(X_{m+n} = j | X_0 = i) \\
&= \sum_{k \in \mathfrak{X}} \mathrm{P}(X_{m+n} = j, X_m = k | X_0 = i) \\
&= \sum_{k \in \mathfrak{X}} \mathrm{P}(X_m = k | X_0 = i) \mathrm{P}(X_{m+n} = j | X_m = k, X_0 = i) \\
&= \sum_{k \in \mathfrak{X}} \mathrm{P}(X_m = k | X_0 = i) \mathrm{P}(X_{m+n} = j | X_m = k) \quad (\because \text{ Markov}) \\
&= \sum_{k \in \mathfrak{X}} P_{ik}^{(m)} P_{kj}^{(n)}
\end{aligned}$$

Chapman-Kolmogorov Equation in Matrix Notation

For $n = 1, 2, 3, \ldots$, let

$$\mathbb{P}^{(n)} = \begin{pmatrix} P_{00}^{(n)} & P_{01}^{(n)} & P_{02}^{(n)} & \cdots & P_{0j}^{(n)} & \cdots \\ P_{10}^{(n)} & P_{11}^{(n)} & P_{12}^{(n)} & \cdots & P_{1j}^{(n)} & \cdots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \ddots \\ P_{i0}^{(n)} & P_{i1}^{(n)} & P_{i2}^{(n)} & \cdots & P_{ij}^{(n)} & \cdots \\ \vdots & \vdots & \vdots & \ddots & \vdots & \ddots \end{pmatrix}$$

be the n-step transition probability matrix.

The Chapman-Kolmogorov equation just asserts that

$$\mathbb{P}^{(m+n)} = \mathbb{P}^{(m)} \times \mathbb{P}^{(n)}$$

Note $\mathbb{P}^{(1)} = \mathbb{P}$, $\Rightarrow \mathbb{P}^{(2)} = \mathbb{P}^{(1)} \times \mathbb{P}^{(1)} = \mathbb{P} \times \mathbb{P} = \mathbb{P}^2$.

By induction,

$$\mathbb{P}^{(n)} = \mathbb{P}^{(n-1)} \times \mathbb{P}^{(1)} = \mathbb{P}^{n-1} \times \mathbb{P} = \mathbb{P}^n$$

Define $\pi_n(i) = \mathrm{P}(X_n = i)$, $i \in \mathfrak{X}$ to be the marginal distribution of X_n, $n = 1, 2, \ldots$. Then again by the law of total probabilities,

$$\begin{aligned}\pi_n(j) &= \mathrm{P}(X_n = j) \\ &= \sum_{k \in \mathfrak{X}} \mathrm{P}(X_0 = k)\mathrm{P}(X_n = j | X_0 = k) \qquad (1) \\ &= \sum_{k \in \mathfrak{X}} \pi_0(k) P_{kj}^{(n)}\end{aligned}$$

Suppose the state space $\mathfrak{X}$ is $\{0, 1, 2, \ldots\}$.
If we write the marginal distribution of X_n as a row vector

$$\pi_n = (\pi_n(0), \pi_n(1), \pi_n(2), \ldots),$$

then the equation (1) is

$$\pi_n = \pi_0 \mathbb{P}^{(n)} = \pi_0 \mathbb{P}^n$$

Example: Ehrenfest Model, 4 Balls

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

Q3 Find $P_{4,2}^{(4)} = \mathrm{P}(X_4 = 2 | X_0 = 4)$.

Q4 Find $P_{4,2}^{(10)} = \mathrm{P}(X_{10} = 2 | X_0 = 4)$.

Q5 Given $\mathrm{P}(X_0 = i) = 1/5$ for $i = 0, 1, 2, 3, 4$, find $\mathrm{P}(X_4 = 2)$

Q6 Find $\mathrm{P}(X_{10} = 2, X_k \geq 2, \text{ for } 1 \leq k \leq 9 | X_0 = 4)$

$$\mathbb{P}^2 = \mathbb{P} \times \mathbb{P} = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{ccccc} 0 & 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} 1/4 & 0 & 3/4 & 0 & 0 \\ 0 & 5/8 & 0 & 3/8 & 0 \\ 1/8 & 0 & 3/4 & 0 & 1/8 \\ 0 & 3/8 & 0 & 5/8 & 0 \\ 0 & 0 & 3/4 & 0 & 1/4 \end{pmatrix} \end{array}$$

$$\mathbb{P}^3 = \mathbb{P} \times \mathbb{P}^2 = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{ccccc} 0 & 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} 0 & 5/8 & 0 & 3/8 & 0 \\ 5/32 & 0 & 3/4 & 0 & 3/32 \\ 0 & 1/2 & 0 & 1/2 & 0 \\ 3/32 & 0 & 3/4 & 0 & 5/32 \\ 0 & 3/8 & 0 & 5/8 & 0 \end{pmatrix} \end{array}$$

$$\mathbb{P}^4 = \mathbb{P}^2 \times \mathbb{P}^2 = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{ccccc} 0 & 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} 5/32 & 0 & 3/4 & 0 & 3/32 \\ 0 & 17/32 & 0 & 15/32 & 0 \\ 1/8 & 0 & 3/4 & 0 & 1/8 \\ 0 & 15/32 & 0 & 5/32 & 0 \\ 3/32 & 0 & 3/4 & 0 & 5/32 \end{pmatrix} \end{array}$$

Example: Ehrenfest Model, 4 Balls (Cont'd)

$$\mathbb{P}^4 = \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{ccccc} 0 & 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} 5/32 & 0 & 3/4 & 0 & 3/32 \\ 0 & 17/32 & 0 & 15/32 & 0 \\ 1/8 & 0 & 3/4 & 0 & 1/8 \\ 0 & 15/32 & 0 & 5/32 & 0 \\ 3/32 & 0 & \boxed{3/4} & 0 & 5/32 \end{pmatrix} \end{array}$$

For Q3, $\mathrm{P}(X_4 = 2 | X_0 = 4) = P_{42}^{(4)} = 3/4.$
which agrees with our previous calculation.

Example: Ehrenfest Model, 4 Balls (Cont'd)

To find $P_{4,2}^{(10)}$ for Q4, it's awful lots of work to compute $\mathbb{P}^{10}$...

There are ways to save some work. By the C-K equation,

$$\mathbb{P}_{4,2}^{(10)} = \underbrace{\mathbb{P}_{4,0}^{(5)}\mathbb{P}_{0,2}^{(5)}}_{=0} + \mathbb{P}_{4,1}^{(5)}\mathbb{P}_{1,2}^{(5)} + \underbrace{\mathbb{P}_{4,2}^{(5)}\mathbb{P}_{2,2}^{(5)}}_{=0} + \mathbb{P}_{4,3}^{(5)}\mathbb{P}_{3,2}^{(5)} + \underbrace{\mathbb{P}_{4,4}^{(5)}\mathbb{P}_{4,2}^{(5)}}_{=0}$$

because it's impossible to move between even states in odd number of moves.

We just need to find $\mathbb{P}_{4,1}^{(5)}$, $\mathbb{P}_{4,3}^{(5)}$, $\mathbb{P}_{1,2}^{(5)}$, and $\mathbb{P}_{3,2}^{(5)}$.

Example: Ehrenfest Model, 4 Balls (Cont'd)

$$\mathbb{P}^5 = \mathbb{P}^2 \times \mathbb{P}^3$$

$$= \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{ccccc} 0 & 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} 1/4 & 0 & 3/4 & 0 & 0 \\ 0 & 5/8 & 0 & 3/8 & 0 \\ 1/8 & 0 & 3/4 & 0 & 1/8 \\ 0 & 3/8 & 0 & 5/8 & 0 \\ 0 & 0 & 3/4 & 0 & 1/4 \end{pmatrix} \end{array} \times \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{ccccc} 0 & 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} 0 & 5/8 & 0 & 3/8 & 0 \\ 5/32 & 0 & 3/4 & 0 & 3/32 \\ 0 & 1/2 & 0 & 1/2 & 0 \\ 3/32 & 0 & 3/4 & 0 & 5/32 \\ 0 & 3/8 & 0 & 5/8 & 0 \end{pmatrix} \end{array}$$

$$= \begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{ccccc} 0 & 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} & & 0 & & \\ & & 3/4 & & \\ & & 0 & & \\ & & 3/4 & & \\ 0 & 15/32 & 0 & 17/32 & 0 \end{pmatrix} \end{array}$$

So

$$\mathbb{P}^{(10)}_{4,2} = \mathbb{P}^{(5)}_{4,1}\mathbb{P}^{(5)}_{1,2} + \mathbb{P}^{(5)}_{4,3}\mathbb{P}^{(5)}_{3,2} = \frac{15}{32} \times \frac{3}{4} + \frac{17}{32} \times \frac{3}{4} = \frac{3}{4}.$$

Example: Ehrenfest Model, 4 Balls (Cont'd)

Q5: Given $\mathrm{P}(X_0 = i) = 1/5$ for $i = 0, 1, 2, 3, 4$, find $\mathrm{P}(X_4 = 2)$.

$$\pi_0 = (\frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}).$$

$$\pi_4 = \pi_0 \mathbb{P}^4 = (\frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}) \begin{pmatrix} 5/32 & 0 & 3/4 & 0 & 3/32 \\ 0 & 17/32 & 0 & 15/32 & 0 \\ 1/8 & 0 & 3/4 & 0 & 1/8 \\ 0 & 15/32 & 0 & 17/32 & 0 \\ 3/32 & 0 & 3/4 & 0 & 5/32 \end{pmatrix}$$

$$\pi_4(2) = (\frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}, \frac{1}{5}) \begin{pmatrix} 3/4 \\ 0 \\ 3/4 \\ 0 \\ 3/4 \end{pmatrix}$$

$$= \frac{1}{5} \cdot \frac{3}{4} + \frac{1}{5} \cdot 0 + \frac{1}{5} \cdot \frac{3}{4} + \frac{1}{5} \cdot 0 + \frac{1}{5} \cdot \frac{3}{4} = \frac{9}{20}$$

Example: Ehrenfest Model, 4 Balls (Cont'd)

Q6: Find $\mathrm{P}(X_{10} = 2, X_k \geq 2,\ \text{for } 1 \leq k \leq 9 | X_0 = 4)$.

Tip: Create another process $\{W_n, n = 0, 1, 2, \dots\}$ with an absorbing state A

$$W_n = \begin{cases} X_n & \text{if } X_k \geq 2 \text{ for all } k = 0, 1, 2, \dots, n \\ A & \text{if } X_k < 2 \text{ for some } k \leq n \end{cases}$$

What is the state space of $\{W_n\}$? $\{A, 2, 3, 4\}$

Is $\{W_n\}$ a Markov chain?

$$W_{n+1} = \begin{cases} A & \text{if } W_n = A \\ W_n + 1 & \text{with prob. } \frac{4-W_n}{4} \text{ if } W_n \neq A \\ W_n - 1 & \text{with prob. } \frac{W_n}{4} \text{ if } W_n = 3 \text{ or } 4 \\ A & \text{with prob. } \frac{W_n}{4} \text{ if } W_n = 2 \end{cases}$$

Yes, $\{W_n\}$ is a Markov chain.

Example: Ehrenfest Model, 4 Balls (Cont'd)

What is the transition probability of $\{W_n\}$?

$$\mathbb{P}_W = \begin{array}{c} \\ A \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccc} A & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 2/4 & 0 & 2/4 & 0 \\ 0 & 3/4 & 0 & 1/4 \\ 0 & 0 & 1 & 0 \end{pmatrix} \end{array}$$

Observe that $\mathbb{P}_{W,i,j}$ equals the transition prob. or the original process $\mathbb{P}_{i,j}$ for $i, j \neq A$.

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

Example: Ehrenfest Model, 4 Balls (Cont'd)

How does $\{W_n\}$ helps us to solve Q6?

$$\text{Observe that } \mathrm{P}(X_{10} = 2, X_k \geq 2, \text{ for } 1 \leq k \leq 9 | X_0 = 4)$$
$$= \mathrm{P}(W_{10} = 2 | W_0 = 4) = P^{(10)}_{W,4,2}$$

It's still an awful lot of work to compute $P^{(10)}_{W,4,2}$.

By the same way we calculate $P^{(10)}_{4,2}$, using C-K equation, we know

$$\mathbb{P}^{(10)}_{W,4,2} = \mathbb{P}^{(5)}_{W,4,A} \underbrace{\mathbb{P}^{(5)}_{W,A,2}}_{=0} + \underbrace{\mathbb{P}^{(5)}_{W,4,2}\mathbb{P}^{(5)}_{W,2,2}}_{=0} + \mathbb{P}^{(5)}_{W,4,3}\mathbb{P}^{(5)}_{W,3,2} + \underbrace{\mathbb{P}^{(5)}_{W,4,4}\mathbb{P}^{(5)}_{W,4,2}}_{=0}$$

in which

- $\mathbb{P}^{(5)}_{W,A,2} = 0$ because $\{W_n\}$ will never leave A.
- $\mathbb{P}^{(5)}_{W,4,2} = \mathbb{P}^{(5)}_{W,4,4} = 0$ because $\{W_n\}$ can never get from 4 to an even numbered state in odd numbers of steps.

Just need to find $\mathbb{P}^{(5)}_{W,4,3}$ and $\mathbb{P}^{(5)}_{W,3,2}$.

Example: Ehrenfest Model, 4 Balls (Cont'd)

$$\mathbb{P}_W^{(2)} = \begin{array}{c} \\ A \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccc} A & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1/2 & 3/8 & 0 & 1/8 \\ 3/8 & 0 & 5/8 & 0 \\ 0 & 3/4 & 0 & 1/4 \end{pmatrix} \end{array}, \quad \mathbb{P}_W^{(3)} = \begin{array}{c} \\ A \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccc} A & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 11/16 & 0 & 5/16 & 0 \\ 3/8 & 15/32 & 0 & 5/32 \\ 3/8 & 0 & 5/8 & 0 \end{pmatrix} \end{array}$$

$$\mathbb{P}_W^{(5)} = \mathbb{P}_W^{(2)} \times \mathbb{P}_W^{(3)} = \begin{array}{c} \\ A \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccc} A & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ & 0 & & \\ & 75/256 & & \\ & 0 & 25/64 & \end{pmatrix} \end{array}$$

So

$$\mathbb{P}_{W,4,2}^{(10)} = \mathbb{P}_{W,4,3}^{(5)} \mathbb{P}_{W,3,2}^{(5)} = \frac{25}{64} \times \frac{75}{256} = \frac{1875}{16384}.$$

For a generalization of Q6, see the discussion starting from the bottom of p.202 to Example 4.14 on p.203 of the 12th edition of the textbook (or p.192-193 of the 11th edition).