n-Step Transition Probabilities:

Consider a Markov chain $\{X_n, n = 0, 1, 2, \ldots\}$, where $X_n \in S$. If $X_0 = i$, then $X_1 = j$ with probability p_{ij}. That is, p_{ij} gives us the probability of going from state i to state j in one step. Now suppose that we are interested in finding the probability of going from state i to state j in two steps, i.e.,

$$p_{ij}^{(2)} = P(X_2 = j | X_0 = i).$$

We can find this probability by applying the law of total probability. In particular, we argue that X_1 can take one of the possible values in S. Thus, we can write

$$\begin{aligned} p_{ij}^{(2)} = P(X_2 = j | X_0 = i) &= \sum_{k \in S} P(X_2 = j | X_1 = k, X_0 = i) P(X_1 = k | X_0 = i) \\ &= \sum_{k \in S} P(X_2 = j | X_1 = k) P(X_1 = k | X_0 = i) \quad \text{(by Markov property)} \\ &= \sum_{k \in S} p_{kj} p_{ik}. \end{aligned}$$

We conclude

$$p_{ij}^{(2)} = P(X_2 = j | X_0 = i) = \sum_{k \in S} p_{ik} p_{kj} \qquad (11.4)$$

We can explain the above formula as follows. In order to get to state j, we need to pass through some intermediate state k. The probability of this event is $p_{ik} p_{kj}$. To obtain $p_{ij}^{(2)}$, we sum over all possible intermediate states. Accordingly, we can define the two-step transition matrix as follows:

$$P^{(2)} = \begin{bmatrix} p_{11}^{(2)} & p_{12}^{(2)} & \ldots & p_{1r}^{(2)} \\ p_{21}^{(2)} & p_{22}^{(2)} & \ldots & p_{2r}^{(2)} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ p_{r1}^{(2)} & p_{r2}^{(2)} & \ldots & p_{rr}^{(2)} \end{bmatrix}.$$

Looking at Equation 11.4, we notice that $p_{ij}^{(2)}$ is in fact the element in the ith row and j th column of the matix

$$P^2 = \begin{bmatrix} p_{11} & p_{12} & \dots & p_{1r} \\ p_{21} & p_{22} & \dots & p_{2r} \\ . & . & . & . \\ . & . & . & . \\ . & . & . & . \\ p_{r1} & p_{r2} & \dots & p_{rr} \end{bmatrix} \cdot \begin{bmatrix} p_{11} & p_{12} & \dots & p_{1r} \\ p_{21} & p_{22} & \dots & p_{2r} \\ . & . & . & . \\ . & . & . & . \\ . & . & . & . \\ p_{r1} & p_{r2} & \dots & p_{rr} \end{bmatrix}.$$

Thus, we conclude that the two-step transition matrix can be obtained by squaring the state transition matrix, i.e.,

$$P^{(2)} = P^2.$$

More generally, we can define the n-step transition probabilities $p_{ij}^{(n)}$ as

$$p_{ij}^{(n)} = P(X_n = j | X_0 = i), \qquad \text{for } n = 0, 1, 2, \cdots, \tag{11.5}$$

and the n-step transition matrix, $P^{(n)}$, as

$$P^{(n)} = \begin{bmatrix} p_{11}^{(n)} & p_{12}^{(n)} & \dots & p_{1r}^{(n)} \\ p_{21}^{(n)} & p_{22}^{(n)} & \dots & p_{2r}^{(n)} \\ . & . & . & . \\ . & . & . & . \\ . & . & . & . \\ p_{r1}^{(n)} & p_{r2}^{(n)} & \dots & p_{rr}^{(n)} \end{bmatrix}.$$

We can now generalize Equation 11.5. Let m and n be two positive integers and assume $X_0 = i$. In order to get to state j in $(m+n)$ steps, the chain will be at some intermediate state k after m steps. To obtain $p_{ij}^{(m+n)}$, we sum over all possible intermediate states:

$$\begin{aligned} p_{ij}^{(m+n)} &= P(X_{m+n} = j | X_0 = i) \\ &= \sum_{k \in S} p_{ik}^{(m)} p_{kj}^{(n)}. \end{aligned}$$

The above equation is called the **Chapman-Kolmogorov equation**. Similar to the case of two-step transition probabilities, we can show that $P^{(n)} = P^n$, for $n = 1, 2, 3, \cdots$.

The Chapman-Kolmogorov equation can be written as

$$\begin{aligned} p_{ij}^{(m+n)} &= P(X_{m+n} = j | X_0 = i) \\ &= \sum_{k \in S} p_{ik}^{(m)} p_{kj}^{(n)}. \end{aligned}$$

The n-step transition matrix is given by

$$P^{(n)} = P^n, \quad \text{for } n = 1, 2, 3, \cdots.$$