APMA1690: Homework # 6 (Due by 11pm on November 2)

1 Review

I would suggest you go through the review section before going to the problem set.

1.1 Notations

- \mathbb{Z} = the collection of all integers.
- $\mathbb{Z}^d = \underbrace{\mathbb{Z} \times \mathbb{Z} \times \cdots \times \mathbb{Z}}_{\text{Cartesian product, } d \text{ times}}$.
- For a Markov chain (MC) $\{X_n\}_{n=0}^{\infty}$, the subscript n is conventionally referred to as "time."
- Let A be a matrix. The transpose of A is denoted as A^{T} .
- Let ${m P}$ be an S-by-S matrix. ${m P}^n = \underbrace{{m P}{m P} \cdots {m P}}_{\text{matrix multiplication, } n \text{ matrices}}$
- $(\mathbf{P}^n)_{ij}$ = the entry in the i^{th} row and j^{th} column of the matrix \mathbf{P}^n .

1.2 Notation ρ_{xy}

Let $\{X_n\}_{n=0}^{\infty}$ be a homogeneous Markov chain taking values in the discrete state space \mathcal{X} , which can be either finite or infinite. Recall that each X_n , for a fixed n, is a random variable, i.e.,

$$X_n: \Omega \to \mathcal{X},$$

 $\omega \mapsto X_n(\omega).$

For the Markov chain and each element $y \in \mathcal{X}$, we define the following random variable

$$T_y(\omega) \stackrel{\text{def}}{=} \min \{ n > 0 \mid X_n(\omega) = y \}$$

= the time at which the sequence $\{ X_n(\omega) \}_{n=1}^{\infty}$ first visits y .

Here, we explicitly write down ω to emphasize that T_y is a random variable. We denote the following probability, which will be used to define "recurrence/transience" and "irreducibility."

$$\rho_{xy} \stackrel{\text{def}}{=} \mathbb{P}(T_y < \infty \mid X_0 = x)$$

= the conditional probability that MC will visit y at least once, given that it starts from x.

1.3 Transition Matrices

Let $\{X_n\}_{n=0}^{\infty}$ be a homogeneous Markov chain whose state space is $\mathcal{X} = \{x_1, x_2, \dots, x_S\}$ (where $S < \infty$) and having transition probability p. We define the following **transition matrix** of the Markov chain

(1.1)
$$P = \begin{pmatrix} p(x_1, x_1) & p(x_1, x_2) & \cdots & p(x_1, x_S) \\ p(x_2, x_1) & p(x_2, x_2) & \cdots & p(x_2, x_S) \\ \vdots & \vdots & \ddots & \vdots \\ p(x_S, x_1) & p(x_S, x_2) & \cdots & p(x_S, x_S) \end{pmatrix}.$$

It is straightforward that $\sum_{j=1}^{S} \mathbf{P}_{ij} = \sum_{j=1}^{S} p(x_i, x_j) = 1$ for all $i \in \{1, 2, \dots, S\}$.

1.4 Irreducibility

Definition 1.1. Let $\{X_n\}_{n=0}^{\infty}$ is a homogeneous Markov chain taking values in the discrete state space \mathcal{X} and having transition probability p.

- 1. The Markov chain $\{X_n\}_{n=0}^{\infty}$ or transition probability p is said to be **recurrent** if all states of \mathcal{X} are recurrent for this Markov chain.
- 2. The Markov chain $\{X_n\}_{n=0}^{\infty}$ or transition probability p is said to be **irreducible** if $\rho_{xy} > 0$ for all $x, y \in \mathcal{X}$, i.e., we have a positive probability of transiting between any two states.

Because of the following theorem, the scenario where the state space \mathcal{X} is finite is of importance in the Markov chain theory.

Theorem 1.1. Let $\{X_n\}_{n=0}^{\infty}$ be a homogeneous Markov chain taking values in the state space \mathcal{X} . If \mathcal{X} is finite, we have

- 1. \mathcal{X} has at least one state that is recurrent for $\{X_n\}_{n=0}^{\infty}$;
- 2. furthermore, if $\{X_n\}_{n=0}^{\infty}$ is irreducible, then $\{X_n\}_{n=0}^{\infty}$ is recurrent, i.e., all states in \mathcal{X} are recurrent for $\{X_n\}_{n=0}^{\infty}$.

1.5 Stationary Distributions

Definition 1.2. Let $\{X_n\}_{n=0}^{\infty}$ be a homogeneous Markov chain taking values in the discrete state space \mathcal{X} and having transition probability p. If a PMF π defined on \mathcal{X} (i.e., $\pi: \mathcal{X} \to [0,1]$) satisfies the following equation,

(1.2)
$$\pi(x) = \sum_{y \in \mathcal{X}} \pi(y) \cdot p(y, x), \quad \text{for all } x \in \mathcal{X},$$

the PMF π is called a stationary distribution or invariant distribution for $\{X_n\}_{n=0}^{\infty}$.

Generally, for a given transition probability p, the existence and uniqueness of a stationary distribution π satisfying Eq. (1.2) are not guaranteed and not trivial. For example, simple random walks taking values in \mathbb{Z}^d do not have a stationary distribution. The general theory of the existence and uniqueness of stationary distributions is sort of complicated (Durrett, 2010, Section 6.5).

When the state space \mathcal{X} is finite, the existence and uniqueness of the stationary distribution of an irreducible Markov chain are crystal clear and easy, which are presented in the following theorem and follow from the "irreducible non-negative matrices version" of the Perron-Frobenius theorem in linear algebra (Meyer, 2000, Section 8.3).

Theorem 1.2. Let $P = (p(x_i, x_j))_{1 \le i,j \le S}$ be the transition matrix of a homogeneous Markov chain $\{X_n\}_{n=0}^{\infty}$ taking values in a finite state space $\mathcal{X} = \{x_1, x_2, \dots, x_S\}$. If the Markov chain $\{X_n\}_{n=0}^{\infty}$ is irreducible, this chain has a unique stationary distribution on \mathcal{X} , i.e., $\pi(x) = \sum_{y \in \mathcal{X}} \pi(y) \cdot p(y, x)$, for all $x \in \mathcal{X}$; equivalently,

$$\boldsymbol{\pi}^{\mathsf{T}} = \boldsymbol{\pi}^{\mathsf{T}} \boldsymbol{P},$$

where $\boldsymbol{\pi} = (\pi(x_1), \dots, \pi(x_S))^{\mathsf{T}}$. Furthermore, $\pi(x_i) > 0$ for all $i = 1, \dots, S$.

1.6 Directed Graphs

Definition 1.3. For the transition matrix P of a homogeneous Markov chain taking values in $\mathcal{X} = \{x_1, \dots, x_S\}$, we define the **directed graph** G(P) = (V, E) **for** P as follows

- 1. The collection of vertices of the graph is $V = \{x_1, \dots, x_S\}$;
- 2. The collection of directed edges of the graph is E, and the directed edge $(x_i \to x_j) \in E$ if and only if $P_{ij} = p(x_i, x_j) > 0$.

The following example helps you get familiar with the definition above. Consider the following transition probability matrix

(1.4)
$$\mathbf{P} = \begin{pmatrix} 0.3 & 0 & 0 & 0.70 & 0 & 0 \\ 0.1 & 0.2 & 0.3 & 0.4 & 0 & 0 & 0 \\ 0 & 0 & 0.5 & 0.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.5 & 0 & 0.5 & 0 \\ 0.6 & 0 & 0 & 0 & 0.4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.2 & 0.8 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}.$$

The directed graph G(P) associated with the P is the one in Figure 1.

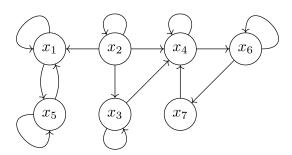


Figure 1: The directed graph G(P), where P is the one defined in Eq. (1.4).

Definition 1.4. Let $G(\mathbf{P})$ be the directed graph defined in Definition 1.3. For two given vertices $x, y \in V$, we say that there exists a directed path going from x to y, if there exist finitely many vertices, say $\xi^{(1)}, \xi^{(2)}, \ldots, \xi^{(l)}$, such that the following conditions are satisfied

- $\xi^{(1)}, \xi^{(2)}, \dots, \xi^{(l)} \in V$;
- the directed edges $(x \to \xi^{(1)}), (\xi^{(1)} \to \xi^{(2)}), (\xi^{(2)} \to \xi^{(3)}), \dots, (\xi^{(l-1)} \to \xi^{(l)}), (\xi^{(l)} \to y)$ belong to E.

The collection $\{(x \to \xi^{(1)}), (\xi^{(1)} \to \xi^{(2)}), (\xi^{(2)} \to \xi^{(3)}), \dots, (\xi^{(l-1)} \to \xi^{(l)}), (\xi^{(l)} \to y)\}$ of directed edges is called a path going from x to y.

For example, in Figure 1, $\{(x_2 \to x_3), (x_3 \to x_4)\}$ is a directed path going from x_2 to x_4 .

Theorem 1.3. Let P be the transition matrix of a homogeneous Markov chain taking values in the state space $\mathcal{X} = \{x_1, \dots, x_S\}$. The Markov chain is irreducible if and only if G(P) satisfies the following: for each pair of vertices x_i and x_j , there exist at least one directed path going from x_i to x_j and one directed path going from x_j to x_i .

The proof of Theorem 1.3 is left as a homework question.

1.7 Asymptotic Theorems

Theorem 1.4. Let $\{X_n\}_{n=0}^{\infty}$ be a homogeneous Markov chain taking values in a finite state space $\mathcal{X} = \{x_1, \ldots, x_S\}$. If this Markov chain is **irreducible** and **aperiodic**, we have

(1.5)
$$\lim_{n \to \infty} \mathbb{P}(X_n = x_j \mid X_0 = x_i) = \pi(x_j) \quad \text{for all } i, j \in \{1, \dots, S\}, \quad \text{equivalently}$$
$$\lim_{n \to \infty} (\mathbf{P}^n)_{ij} = \pi(x_j) \quad \text{for all } i, j \in \{1, \dots, S\},$$

where π is the unique stationary distribution of the Markov chain.

Theorem 1.5 further implies the following

$$\lim_{n \to \infty} \mathbb{P}(X_n = x_j) = \sum_{i=1}^{S} \left[\lim_{n \to \infty} \mathbb{P}(X_n = x_j \mid X_0 = x_i) \right] \cdot \mathbb{P}(X_0 = x_i)$$

$$= \pi(x_j) \cdot \sum_{i=1}^{S} \mathbb{P}(X_0 = x_i)$$

$$= \pi(x_j), \quad \text{for all } j = 1, \dots, S,$$

that is, X_n looks like a π -distributed random variable when n is sufficiently large.

Theorem 1.5. Let $\{X_n\}_{n=0}^{\infty}$ be a homogeneous Markov chain taking values in a finite state space \mathcal{X} . If this chain is irreducible, for any function $f: \mathcal{X} \to \mathbb{R}$ such that $\sum_{x \in \mathcal{X}} |f(x)| \cdot \pi(x) < \infty$, we have

(1.6)
$$\lim_{n \to \infty} \left\{ \frac{1}{n} \sum_{i=1}^{n} f(X_i) \right\} = \sum_{x \in \mathcal{X}} f(x) \cdot \pi(x), \quad \text{with probability one,}$$

where π is the stationary of $\{X_n\}_{n=0}^{\infty}$.

The "with probability one" in Eq. (1.6) means the following

$$\mathbb{P}\left\{\omega \in \Omega \left| \lim_{n \to \infty} \left[\frac{1}{n} \sum_{i=1}^{n} f\left(X_{i}(\omega)\right) \right] = \sum_{x \in \mathcal{X}} f(x) \cdot \pi(x) \right\} = 1.$$

2 Problem Set

1. (2 points) Prove Theorem 1.3 (see the Review section).

Theorem 1.3 claims that a finite Markov Chain is irreducible iff its directed graph has as least one directed path from $x_i \to x_j$ and at least one from $x_j \to x_i$ for every pair of vertices (x_i, x_j) .

If the MC is irreducible, then for any states x_i, x_j

$$\rho_{x_i,x_j} > 0$$

i.e., there is a non-zero probability of eventually reaching x_i , starting at x_j . Equivalently, there is a path from x_j to x_i . Similarly, since x_i and x_j are arbitrary, $\rho_{x_j,x_i} > 0$. Thus, we have a path in the directed graph from any point x_i to x_j and vice versa.

The proof of the other direction, is practically the same. If there exist edges in the directed graph, then $p(x_i, x_j) > 0$ and $p(x_j, x_i) > 0$ so $\rho_{x_i, x_j} > 0$ and $\rho_{x_j, x_i} > 0$.d Then as these points are arbitrary, the MC is irreducible.

2. (3 points) In this question, you will be asked to provide a partial proof for Theorem 1.2. By solving this problem, you will observe how algebraic topology (MATH 2410, Hatcher (2002)), linear algebra, and probability theory intersect.

We first state a generalized version of the Brouwer fixed-point theorem, which is a result in algebraic topology:

Theorem 2.1 (generalized Brouwer fixed-point theorem). Let $K \subset \mathbb{R}^S$ be convex, bounded, and closed. Every continuous function $f: K \to K$ has a fixed point, i.e., there exists $x \in K$ such that f(x) = x.

(Notice: To use the Brouwer fixed-point theorem, you have to verify that $f(K) \subset K$, i.e., $f(\xi) \in K$ for all $\xi \in K$.)

Please assume that Theorem 2.1 is true and apply it to show the following:

Let $P = (p(x_i, x_j))_{1 \le i, j \le S}$ be the transition matrix of a homogeneous Markov chain $\{X_n\}_{n=0}^{\infty}$ taking values in a finite state space $\mathcal{X} = \{x_1, x_2, \dots, x_S\}$. Then, there exists $\pi \in \Delta$ such that $P^{\mathsf{T}}\pi = \pi$, where

$$\Delta = \left\{ oldsymbol{\xi} = (\xi_1, \dots, \xi_S)^\intercal \in \mathbb{R}^S \, \middle| \, \sum_{i=1}^S \xi_i = 1 \, \, ext{and} \, \, \xi_i \geq 0 \, \, ext{for all} \, \, i = 1, 2, \dots, S
ight\}.$$

Furthermore, if all entries of P are positive, i.e., $p(x_i, x_j) > 0$ for all i and j, all entries of the vector π are positive.

Hint: Apply Theorem 2.1 by letting $K = \Delta$ and $f(\xi) = \mathbf{P}^{\mathsf{T}} \xi$. In your proof, you do not need to show that $K = \Delta$ is bounded and closed, which might be outside the scope of APMA 1690. But you need to show that $K = \Delta$ is convex (see the definition of convex sets by clicking the link).

Remark: Here, we assume all entries of P are strictly positive. To remove the strict positivity condition, we need the irreducibility of the Markov chain. In addition, this question does not involve the uniqueness of π . The uniqueness needs the the irreducibility structure. The set Δ defined above is usually referred to as the **probability simplex**, which is a fundamental building block of the simplicial homology theory in algebraic topology.

Consider the probability simplex

$$\Delta = \left\{ \boldsymbol{\xi} = (\xi_1, \dots, \xi_S)^{\mathsf{T}} \in \mathbb{R}^S \,\middle|\, \sum_{i=1}^S \xi_i = 1 \text{ and } \xi_i \ge 0 \text{ for all } i = 1, 2, \dots, S \right\}.$$

We assume the space is bounded and closed. To see that it is convex, observe that for $x, y \in \Delta$,

$$(1-t)x + ty \in \Delta$$
 $t \in [0,1]$

because

$$(1-t)\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_S \end{pmatrix} + t \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_S \end{pmatrix} = \begin{pmatrix} x_1 - t(x_1 - y_1) \\ x_2 - t(x_2 - y_2) \\ \vdots \\ x_S - t(x_S - y_S) \end{pmatrix}$$

and

$$\sum_{i=1}^{S} x_i - t(x_i - y_i) = \sum_{x=1}^{S} x_i - \sum_{i=1}^{S} t(x_i - y_i)$$

$$= 1 - t \left(t \sum_{i=1}^{S} x_i - \sum_{i=1}^{S} y_i \right)$$

$$= 1 - t(1 - 1)$$

$$= 1$$

To see the second condition, observe that x_i, y_i, t are all ≥ 0 so

$$x_1 - t(x_1 - y_1) = x_1 - tx_1 + ty_1$$

and so with t=0, we have $x_1 \geq 0$ and t=1, we have $y_1 \geq 0$ so $(1-t)x+ty \in \Delta$. Thus, the probability simplex fits the conditions of the Brouwer fixed-point theorem. Now consider $f(\vec{\xi}) = P^T \vec{\xi}$ where $\vec{\xi} \in \Delta$:

$$f(\vec{\xi}) = \begin{pmatrix} p(x_1, x_1) & p(x_2, x_1) & \dots & p(x_S, x_1) \\ p(x_1, x_2) & p(x_2, x_2) & \dots & p(x_S, x_2) \\ \vdots & \vdots & \ddots & \vdots \\ p(x_1, x_S) & p(x_2, x_S) & \dots & p(X_S, x_S) \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \\ \vdots \\ \xi_S \end{pmatrix}$$

$$= \begin{pmatrix} \sum_{i=1}^S \xi_i \cdot p(x_i, x_1) \\ \sum_{i=1}^S \xi_i \cdot p(x_i, x_2) \\ \vdots \\ \sum_{i=1}^S \xi_i \cdot p(x_i, x_S) \end{pmatrix}$$

Clearly, this is a vector in \mathbb{R}^S and further,

$$\sum_{j=1}^{S} \sum_{i=1}^{S} \xi_{i} \cdot p(x_{i}, x_{j}) = \sum_{i=1}^{S} \sum_{j=1}^{S} \xi_{i} \cdot p(x_{i}, x_{j})$$

$$= \sum_{i=1}^{S} \xi_{i} \sum_{j=1}^{S} \cdot p(x_{i}, x_{j})$$

$$= \sum_{i=1}^{S} \xi_{i} \sum_{j=1}^{S} \cdot p(x_{i}, x_{j})$$

$$= \sum_{i=1}^{S} \xi_{i} \cdot 1$$

$$= 1$$

Then because $0 \le p(x_i, x_j)$ and $\xi_i \ge 0$, every entry in the vector will be a sum of strictly non-negative terms so the entries themselves will be non-negative. Thus, $f(\Delta) \subset \Delta$.

Then by the Brouwer fixed point theorem, there exists $\pi \in \Delta$ such that $f(\pi) = P^T \vec{\pi} = \vec{\pi}$. Finally, if all entries of P are strictly positive, then each entry of π will be of the form

$$\pi(x_i) = \sum_{i=1}^{S} p(x_j, x_i) \cdot \pi(x_i)$$

But since we already know $\vec{\pi} \in \Delta$,

$$\sum_{I=1}^{S} \pi(x_i) = 1$$

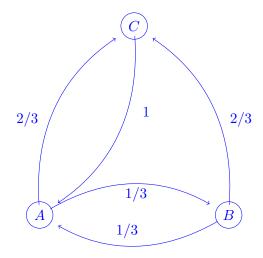
which means that at least one $\{\pi(x_i)\}_{i=1}^S$ must be positive and none of them can be negative. So the sum $\sum_{i=1}^S p(x_j, x_i) \cdot \pi(x_i)$ must be positive.

3. Suppose $\{X_n\}_{n=0}^{\infty}$ is a homogeneous Markov chain taking values in the state space $\mathcal{X} = \{x_1, x_2, x_3\}$, and its transition probability matrix is the following

$$\mathbf{P} = \begin{pmatrix} 0 & 1/3 & 2/3 \\ 1/3 & 0 & 2/3 \\ 1 & 0 & 0 \end{pmatrix}.$$

(a) (1 point) Prove that the Markov chain $\{X_n\}_{n=0}^{\infty}$ is irreducible. (Hint: You may use Theorem 1.3.)

The directed graph of P can be represented



Notice that there is a path from every node to every other node (A and B are trivial and $C \to A \to B$). Thus, by theorem 1.3, P is irreducible.

(b) (1 point) Prove that the Markov chain $\{X_n\}_{n=0}^{\infty}$ is aperiodic. The period of a Markov chain is given by $d = \gcd(I_i)$ where $I_i = \{n \ge 1 \mid (P^n)_{ii} > 0\}$. We calculate the first few powers:

$$P^{2} = \begin{pmatrix} 7/9 & 0 & 2/9 \\ 6/9 & 1/9 & 2/9 \\ 0 & 3/9 & 6/9 \end{pmatrix}$$

$$P^{3} = \begin{pmatrix} 2/9 & 7/27 & 14/27 \\ 7/27 & 2/9 & 14/27 \\ 7/9 & 0 & 2/9 \end{pmatrix}$$

And see that both $2 \in I_i$ and $3 \in I_i$ for $i = \{1, 2, 3\}$ because both main diagonals are positive. But 2 and 3 are already coprime so no matter what other values are in I_i , the GCD is 1 and the MC is aperiodic.

(c) (1 point) Compute the stationary distribution of the Markov chain $\{X_n\}_{n=0}^{\infty}$. By Theorem 1.2, as the MC is irreducible, its unique stationary distribution is given by $\vec{\pi}^T = \vec{\pi}^T P$

$$(\pi(x_1) \quad \pi(x_2) \quad \pi(x_3)) = (\pi(x_1) \quad \pi(x_2) \quad \pi(x_3)) \begin{pmatrix} 0 & 1/3 & 2/3 \\ 1/3 & 0 & 2/3 \\ 1 & 0 & 0 \end{pmatrix}$$

$$= (\frac{1}{3}\pi(x_1) + \pi(x_3) \quad \frac{1}{3}\pi(x_1) \quad \frac{2}{3}\pi(x_1) + \frac{2}{3}\pi(x_2))$$

Which gives a system we can put in terms of $\pi(x_1)$:

$$\begin{cases} \pi(x_1) = \frac{1}{3}\pi(x_1) + \pi(x_3) \\ \pi(x_2) = \frac{1}{3}\pi(x_1) \\ \pi(x_3) = \frac{2}{3}\pi(x_1) + \frac{2}{3}\pi(x_2) \end{cases} = \begin{cases} \pi(x_1) = \pi(x_1) \\ \pi(x_2) = \frac{1}{3}\pi(x_1) \\ \pi(x_3) = \frac{2}{3}\pi(x_1) + \frac{2}{9}\pi(x_1) = \frac{8}{9}\pi(x_1) \end{cases}$$

Further, we have that

$$\pi(x_1) + \pi(x_2) + \pi(x_3) = 1$$

so

$$\pi(x_1) + \frac{1}{3}\pi(x_1) + \frac{8}{9}\pi(x_1) = \frac{20}{9}\pi(x_1) = 1 \implies \pi(x_1) = \frac{9}{20}$$

Substituting back in,

$$\begin{cases} \pi(x_1) = \frac{9}{20} \\ \pi(x_2) = \frac{1}{3} \cdot \frac{9}{20} = \frac{3}{20} \\ \pi(x_3) = \frac{8}{9} \cdot \frac{9}{20} = \frac{8}{20} \end{cases}$$

so

$$\vec{\pi}^T = \begin{pmatrix} 9/20 \\ 3/20 \\ 2/5 \end{pmatrix}$$

(d) (1 point) Suppose the function $f: \mathcal{X} \to \mathbb{R}$ is defined as follows

$$f(x_k) = k^2$$
, for all $k = 1, 2, 3$.

Compute the following value.

$$\sum_{x \in \mathcal{X}} f(x) \cdot \pi(x),$$

where π is the stationary distribution you derived in part (c).

$$\sum_{x \in \mathfrak{X}} f(x) \cdot \pi(x) = f(x_1) \cdot \pi(x_1) + f(x_2) \cdot \pi(x_2) + f(x_3) \cdot \pi(x_3)$$

$$= 1 \cdot \frac{9}{20} + 4 \cdot \frac{3}{20} + 9 \cdot \frac{2}{5}$$

$$= \frac{9 + 12 + 72}{20}$$

$$= \left\lceil \frac{93}{20} \right\rceil$$

(e) (1 point) Compute the following limit

$$\lim_{n\to\infty} \boldsymbol{P}^n.$$

(Hint: the limit is a 3-by-3 matrix.)

Since the MC is irreducible and aperiodic, we can apply Theorem 1.4:

$$\lim_{n \to \infty} P^n = \begin{pmatrix} \pi(x_1) & \pi(x_2) & \pi(x_3) \\ \pi(x_1) & \pi(x_2) & \pi(x_3) \\ \pi(x_1) & \pi(x_2) & \pi(x_3) \end{pmatrix}$$
$$= \begin{pmatrix} 9/20 & 3/20 & 2/5 \\ 9/20 & 3/20 & 2/5 \\ 9/20 & 3/20 & 2/5 \end{pmatrix}$$

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