# Stochastic Simulation APPM 7400

### Lesson 13: Markov Chains

(Discrete Time) October 8, 2018

Lesson 13: Markov Chains

A Markov chain  $\{X_n\}$  is a stochastic process with a sort of "limited memory":

$$P(X_{n+1} = j | X_n = i, X_{n-1} = i_{n-1}, \dots, X_0 = i_0)$$
  
=  $P(X_{n+1} = j | X_n = i)$ 

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Note:

• This does not mean that  $X_{n+1}$  is independent of the earlier  $X_0, X_1, \ldots, X_{n-1}$ .

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$$= P(X_{n+1} = j | X_n = i)$$

Note:

- This does not mean that  $X_{n+1}$  is independent of the earlier  $X_0, X_1, \ldots, X_{n-1}$ .
- Though we can say that  $X_{n+1}$  is "conditionally independent" of  $X_0, X_1, \ldots, X_{n-1}$ , "given  $X_n$ ".

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Note that the Markov property not only implies that (for example)

 $P(X_3 = 4 | X_2 = 0, X_1 = 2, X_0 = 8) = P(X_3 = 4 | X_2 = 0)$ 

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 $P(X_3 = 4 | X_2 = 0, X_1 = 2, X_0 = 8) = P(X_3 = 4 | X_2 = 0)$ 

but also that  $P(X_3 = 4 | X_1 = 2, X_0 = 8) = P(X_3 = 4 | X_1 = 2)$ 

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$$= \sum_{j} P(X_{3} = 4, X_{2} = j | X_{1} = 2, X_{0} = 8)$$

$$= \sum_{j} P(X_{3} = 4 | X_{2} = j, X_{1} = 2, X_{0} = 8) \cdot P(X_{2} = j | X_{1} = 2, X_{0} = 8)$$

$$\stackrel{M.P.}{=} \sum_{j} P(X_{3} = 4 | X_{2} = j) \cdot P(X_{2} = j | X_{1} = 2)$$

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$$= \sum_{j} P(X_{3} = 4, X_{2} = j, X_{1} = 2) = P(X_{3} = 4 | X_{1} = 2)$$

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Example 1:

Suppose that a warehouse stocks a certain item to satisfy a continuing demand. The stock is checked at times  $t_n$ , n > 1.

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At each checking time, if the stock is below some prescribed level a, then the stock is replenished up to some prescribed level b (a < b), otherwise nothing is done.

The demand for the item during the time interval  $[t_{n-1}, t_n)$  is random.

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Example 1 (continued):

For n = 0, 1, ..., let

 $X_n$  = stock level just before time  $t_n$ 

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Then  $\{X_n\}$  is a discrete time stochastic process with (finite) "state space"

 $S = \{0, 1, 2, \dots, b\}$ 

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 $X_n$  = stock level just before time  $t_n$ 

Then  $\{X_n\}$  is a discrete time stochastic process with (finite) "state space"  $S = \{0, 1, 2, ..., b\}$ 

Furthermore,  $\{X_n\}_{n\geq 0}$  is a Markov chain.

Example 2:

Customers arrive at a taxi stand and a taxi arrives every 5 minutes. Assume that a single customer is served during each time period, if there are customers and that the taxi drives away empty if there are no customers. Example 2:

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Assume that the customers are arriving at random times, say

 $Y_n = \#$  arriving during time period n

(Assumed to be iid and independent of the number of customers waiting.)

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Let

 $X_n = \#$  customers waiting at the start of time period n

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Example 2 (continued):

Then  $\{X_n\}_{n\geq 0}$  is a Markov chain with state space  $S = \{0, 1, 2, \ldots\}$ 

Proof:  

$$X_{n+1} = \begin{cases} X_n - 1 + Y_n &, & \text{if } X_n \ge 1 \\ Y_n &, & \text{if } X_n = 0 \end{cases}$$

So, if  $i \geq 1$ ,

$$P(X_{n+1} = j | X_n = i, X_{n-1} = i_{n-1}, \dots, X_0 = i_0)$$
  
=  $P(X_n - 1 + Y_n = j | X_n = i, X_{n-1} = i_{n-1}, \dots, X_0 = i_0)$   
=  $P(Y_n = j - i_n + 1 | X_n = i, X_{n-1} = i_{n-1}, \dots, X_0 = i_0)$ 

 $= P(Y_n = j - i + 1)$ 

by assumption of the independence of the  $\{Y_n\}$  and  $\{X_n\}$  processes.

Example 2 (continued):

Proceeding in the same way, we can get

$$P(X_{n+1} = j | X_n = i) = P(Y_n = j - i + 1)$$

So we see that

$$P(X_{n+1} = j | X_n = i, X_{n-1} = i_{n-1}, \dots, X_0 = i_0) = P(X_{n+1} = j | X_n = i)$$

Warning: It would not have been enough to only show that

$$P(X_{n+1} = j | X_n = i, X_{n-1} = i_{n-1}, \dots, X_0 = i_0)$$

depends only on i and j.

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Note that, since the  $Y_n$  are iid,

$$P(X_{n+1} = j | X_n = i) = P(Y_n = j - i + 1)$$

does not depend on time.

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Note that, since the  $Y_n$  are iid,

$$P(X_{n+1} = j | X_n = i) = P(Y_n = j - i + 1)$$

does not depend on time.

This is a time-homogeneous Markov chain.

In this case we can write

$$p_{ij} = P(X_{n+1} = j | X_n = i)$$

which is the same as

$$P(X_n=j|X_0=i).$$

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For a time-homogeneous Markov chain, say on  $S = \{0, 1, 2, ...\}$ , we can organize transition probabilities into a (one-step) transition probability matrix:



 $\sum_{j\in S} p_{ij} = 1$ 

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Example:

Suppose that items produced by a certain worker in a factory are classified as "defective" or "non-defective".

Further suppose that, due to trends in raw material quality, whether or not a particular item is defective depends, in part, on whether the previous item was defective.

### Example (continued):

### Let

$$X_n = \begin{cases} 0 & , & \text{if } n^{th} \text{ item is not defective} \\ 1 & , & \text{if } n^{th} \text{ item is defective} \end{cases}$$

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### Example (continued):

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$$X_n = \begin{cases} 0 & , & \text{if } n^{th} \text{ item is not defective} \\ 1 & , & \text{if } n^{th} \text{ item is defective} \end{cases}$$

Suppose that the probability transition matrix is

$$\mathcal{P} = \begin{array}{c} 0 & 1 \\ 0.99 & 0.01 \\ 1 & 0.08 & 0.92 \end{array} \right]$$

(This suggests that defective items tend to appear in bunches.)

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### FINITE DIMENSIONAL DISTRIBUTIONS OF DTMCs

Given the probability transition matrix  $\mathcal{P}$ , how do we find

$$P(X_0 = i_0, X_1 = i_1, \dots, X_n = i_n)?$$

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$$P(X_0 = i_0, X_1 = i_1, \dots, X_n = i_n)?$$

The transition matrix describes transitions but we still need a starting (initial) distribution:

Definition:

$$\pi_i = P(X_0 = i)$$

 $(\sum_{i\in S}\pi_i=1)$ 

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Claim: Let  $\{X_n\}$  be a DTMC on a state space S with probability transition matrix  $\mathcal{P} = [p_{ij}]$ .

Then for any  $i_0, i_1, \ldots, i_n \in S$ ,

 $P(X_0 = i_0, X_1 = i_1, \dots, X_n = i_n) = \pi_{i_0} p_{i_0 i_1} p_{i_1 i_2} \cdots p_{i_{n-1} i_n}$ 

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Proof:  $P(X_0 = i_0, X_1 = i_1, \dots, X_n = i_n)$ 

$$= P(X_n = i_n | X_{n-1} = i_{n-1}, \dots, X_0 = i_0) \cdot P(X_{n-1} = i_{n-1}, \dots, X_0 = i_0)$$

$$= P(X_n = i_n | X_{n-1} = i_{n-1}) \cdot P(X_{n-1} = i_{n-1}, \dots, X_0 = i_0)$$

$$= p_{i_{n-1}i_n} \cdot P(X_{n-1} = i_{n-1}, \dots, X_0 = i_0) = \dots =$$

 $= p_{i_{n-1}i_n} \cdot p_{i_{n-2}i_{n-1}} \cdots p_{i_0i_1} \cdot P(X_0 = i_0) = p_{i_{n-1}i_n} \cdot p_{i_{n-2}i_{n-1}} \cdots p_{i_0i_1} \cdot \pi_{i_0}$ 

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### FINITE DIMENSIONAL DISTRIBUTIONS OF DTMCs

What about the distribution of  $X_{n_1}, X_{n_2}, \ldots, X_{n_k}$  for some  $n_1 < n_2 < \cdots < n_k$ ?

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### FINITE DIMENSIONAL DISTRIBUTIONS OF DTMCs

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Just sum (integrate) out the ones you don't want.

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What about the distribution of  $X_{n_1}, X_{n_2}, \ldots, X_{n_k}$  for some  $n_1 < n_2 < \cdots < n_k$ ?

Just sum (integrate) out the ones you don't want.

For the defective factory items example:

Suppose	$\begin{array}{rcl} \pi_0 & = \\ \pi_1 & = \end{array}$	0.89 0.11	$P(X_1 = 1, X_3 = 0) =$ $P(X_0 = 0, X_1 = 1, X_2 = 0, X_3 = 0)$
$\mathcal{P} =$	0.99 0.08	0.01 0.92	$ \begin{aligned} &+P(X_0=1,X_1=1,X_2=0,X_3=0)\\ &+P(X_0=0,X_1=1,X_2=1,X_3=0)\\ &+P(X_0=1,X_1=1,X_2=1,X_3=0) \end{aligned}$

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So,

 $\approx \ 0.0168$ 

+(0.11)(0.92)(0.92)(0.08)

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+(0.89)(0.01)(0.92)(0.08)

+(0.11)(0.92)(0.08)(0.99)

 $P(X_1 = 1, X_3 = 0) = (0.89)(0.01)(0.08)(0.99)$ 

FINITE DIMENSIONAL DISTRIBUTIONS OF DTMCs

Before: 
$$p_{ij} = P(X_{k+1} = j | X_k = i)$$

Now define:  $p_{ij}^{(n)} = P(X_{k+n} = j | X_{k=i})$ 

and write the *n*-step transition matrix:

$$\mathcal{P}^{(n)} = \begin{bmatrix} 0 & 1 & 2 & \cdots \\ p_{00}^{(n)} & p_{01}^{(n)} & p_{02}^{(n)} & \cdots \\ p_{10}^{(n)} & p_{11}^{(n)} & p_{12}^{(n)} & \cdots \\ p_{20}^{(n)} & p_{21}^{(n)} & p_{22}^{(n)} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

(Still a time-homogeneous setting.)

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### Question:

How does the *n*-step transition probability matrix relate to the onestep transition probability matrix?

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Example: Return to Defective Factory Items

Let's find  $P(X_2 = 1 | X_0 = 0)$ .

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Example: Return to Defective Factory Items

Let's find  $P(X_2 = 1 | X_0 = 0)$ .

Given we started at 0, we either went from

 $0 \to 0 \to 1$ 

#### or

#### $0 \to 1 \to 1$
## **n-Step Transition Probabilities**

 $egin{array}{c} 0 
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These paths represent disjoint events. So

 $P(X_2 = 1 | X_0 = 0) = p_{00}p_{01} + p_{01}p_{11}$ 

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## **n-Step Transition Probabilities**

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Look familiar?

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Look familiar?

$$\begin{bmatrix} p_{00} & p_{01} \\ p_{10} & p_{11} \end{bmatrix} \begin{bmatrix} p_{00} & p_{01} \\ p_{10} & p_{11} \end{bmatrix} = \begin{bmatrix} p_{00}p_{00} + p_{01}p_{10} & p_{00}p_{01} + p_{01}p_{11} \\ p_{00}p_{10} + p_{11}p_{10} & p_{10}p_{01} + p_{11}p_{11} \end{bmatrix}$$

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#### Theorem:

The *n*-step transition probability

$$p_{ij}^{(n)} = P(X_{k+n} = j | X_k = i)$$

is the  $ij^{th}$  entry of the  $n^{th}$  power of  $\mathcal{P}$ .

 $\mathcal{P}^{(n)} = \mathcal{P}^n$ 

(Though  $p_{ij}^{(n)} \neq p_{ij}^{n}$ .)

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### FINITE DIMENSIONAL DISTRIBUTIONS OF DTMCs

To prove this, we need the

Chapman-Kolmogorov Equations  $p_{ij}^{(m+n)} = \sum_{k \in S} p_{ik}^{(m)} \cdot p_{kj}^{(n)}$ 

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To prove this, we need the

Chapman-Kolmogorov Equations  $p_{ij}^{(m+n)} = \sum_{k \in S} p_{ik}^{(m)} \cdot p_{kj}^{(n)}$ 

Then the theorem is proven since

$$p_{ij}^{(m+1)} = \sum_{k \in S} p_{ik}^{(m)} \cdot p_{kj}$$

is the  $ij^{th}$  entry of  $\mathcal{P}^{(m)} \cdot \mathcal{P}$ .

$$p_{ij}^{(m+n)} = P(X_{m+n} = j | X_0 = i)$$

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$$p_{ij}^{(m+n)} = P(X_{m+n} = j | X_0 = i)$$
  
=  $\sum_{k \in S} P(X_{m+n} = j, X_n = k | X_0 = i)$ 

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$$p_{ij}^{(m+n)} = P(X_{m+n} = j | X_0 = i)$$

$$= \sum_{k \in S} P(X_{m+n} = j, X_n = k | X_0 = i)$$

$$= \sum_{k \in S} P(X_{m+n} = j | X_n = k, X_0 = i) \cdot P(X_n = k | X_0 = i)$$

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$$p_{ij}^{(m+n)} = P(X_{m+n} = j | X_0 = i)$$

$$= \sum_{k \in S} P(X_{m+n} = j, X_n = k | X_0 = i)$$

$$= \sum_{k \in S} P(X_{m+n} = j | X_n = k, X_0 = i) \cdot P(X_n = k | X_0 = i)$$

$$\stackrel{M.P.}{=} \sum_{k \in S} P(X_{m+n} = j | X_n = k) \cdot P(X_n = k | X_0 = i)$$

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Consider a MC on  $S = \{0, 1, 2, 3\}$  with transition probability matrix

$$P = \begin{bmatrix} 0 & 1 & 2 & 3 \\ 0.2 & 0.8 & 0 & 0 \\ 1 \\ 2 \\ 3 \end{bmatrix} \begin{bmatrix} 0.2 & 0.8 & 0 & 0 \\ 0.5 & 0.2 & 0.1 & 0.2 \\ 0.2 & 0.1 & 0.6 & 0.1 \\ 0 & 0 & 0.7 & 0.3 \end{bmatrix}$$

Suppose that we start the chain in state 1 and that we stop observing the chain when it first hits state 3.

### Question 1:

What is the expected number of steps the chain will take before stopping?

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Let  $T = \min\{n \ge 0 : X_n = 3\}$ . (*T* is a "first hitting time".)

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Let's define

 $u_i = \mathsf{E}[T|X_0 = i].$ 

Then we want to find  $u_1$ .

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 $\left[\begin{array}{cccccc} 0.2 & 0.8 & 0 & 0 \\ 0.5 & 0.2 & 0.1 & 0.2 \\ 0.2 & 0.1 & 0.6 & 0.1 \\ 0 & 0 & 0.7 & 0.3 \end{array}\right]$ 

 $u_1 = 1 + 0.5u_0 + 0.2u_1 + 0.1u_2 + 0.2(0)$ 

$$u_0 = 1 + 0.2u_0 + 0.8u_1$$

 $u_2 = 1 + 0.2u_0 + 0.1u_1 + 0.6u_2 + (0.1)(0)$ 

 $\begin{array}{rcl} & u_0 &\approx& 9.861 \\ \Rightarrow & u_1 &\approx& 8.610 \\ & u_2 &\approx& 9.583 \end{array}$ 

 $u_i = \mathsf{E}[T|X_0 = i]$ 

#### Pseudocode:

```
steps = 0
state = 1
while (state is not 3)
  uniform = a random number
  cdf = 0
  do i=1,3
    if(uniform < cdf+P(state,I)
     state = I
     exit I loop
    else
     cdf = cdf + P(state,I)
    end if
  end do
  steps = steps + 1
end while
```

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I simulated:

- 100,000 reps starting in state 0
- 100,000 reps starting in state 1
- 100,000 reps starting in state 2

Results:

û <sub>0</sub>	$\approx$	9.866239
$\hat{u}_1$	$\approx$	8.615456
û <sub>2</sub>	$\approx$	9.605806

A really strong form of stability that one might require of a Markov chain  $\{X_n\}$ , is that the distribution of  $X_n$  does not change in time.

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### Definition:

A stochastic process is said to be stationary if, for any  $k \in \mathbb{Z}$ , the distribution of  $(X_n, X_{n+1}, \dots, X_{n+k})$  does not change as *n* varies.

It is clear that, for a stationary process, the distribution of  $X_n$  does not change in time.

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It is clear that, for a stationary process, the distribution of  $X_n$  does not change in time.

On the other hand, for a time-homogeneous Markov chain, if the distribution of  $X_n$  does not change in time, then the process is stationary.

We will call this common distribution  $\pi$ .

ie:

$$\pi_i := P(X_n = i), \qquad i \in S$$

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We will refer to  $\pi$  as the stationary or invariant distribution for the Markov chain.

("Invariant" refers to time invariance.)

Note that:

$$\pi_j = \sum_{i \in S} \pi_i \, \rho_{ij}$$
$$\left(\pi(j) = \sum_{i \in S} \pi(i) \, \rho(i, j)\right)$$

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For a **continuous state space**, if  $\pi$  is the stationary distribution for a MC with "transition law" *P*,  $\pi$  satisfies:

$$\pi(A) = \int_{S} \pi(x) P(x, A) \, dx$$

Here, P(x, A) is the probability that, starting at x, we move into set A in the next time step.

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- For any continuous density f(x), we are using the notation  $f(A) = \int_A f(x) dx$ . So,  $\pi(A) = \int_A \pi(x) dx$ .
- We will assume that  $P(x, A) = \int_A p(x, y) dy$  for some "transition density" p(x, y).

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For the moment, we will assume that  $\pi$  exists and is unique...

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The key thing about the stationary distribution is that, if we start a chain according to a draw from it, and iterate forward according to the transition law P, the chain will maintain that distribution at all fixed time points.

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The key thing about the stationary distribution is that, if we start a chain according to a draw from it, and iterate forward according to the transition law P, the chain will maintain that distribution at all fixed time points.

### ie: $X_0 \sim \pi \quad \Rightarrow \quad X_n \sim \pi \quad \forall n > 0$

If we don't know  $\pi$ , we can't run a sample path of the Markov chain in "stationary mode" because we don't know how to choose a starting value according to  $\pi$ .

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We could then think of the end value of the sample path as a draw from  $\boldsymbol{\pi}.$
What if we start with some arbitrary  $X_0$  and run a sample path for a really long time until we are convinced that the path couldn't possibly remember where it started...

We could then think of the end value of the sample path as a draw from  $\boldsymbol{\pi}.$ 

In fact, we will get the distribution  $\boldsymbol{\pi}$  in the limit:

$$\lim_{n\to\infty}p^{(n)}(x,y)=\pi(y)$$

(If the limit exists.)

Proof:

• Suppose we start the chain according to some distribution  $\varphi$ .

ie: 
$$\varphi_i = P(X_0 = i)$$

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We continue the proof in the continuous setting since it is more general...

(Note that  $\varphi$  could be concentrated at one point.)

• Now suppose that there is a limiting distribution:

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 $P_{\varphi}(X_n \in A) \to \gamma_{\varphi}(A)$ 

for some probability measure  $\gamma_{\varphi}(\cdot)$ .

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Proof (continued): Then,

 $\gamma_{\varphi}(A) = \lim_{n \to \infty} P_{\varphi}(X_n \in A)$ 

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=  $\lim_{n \to \infty} \int \varphi(x) P^{(n)}(x, A) dx$ 

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Proof (continued): Then,

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$$= \lim_{n \to \infty} \int \varphi(x) P^{(n)}(x, A) dx$$
$$= \lim_{n \to \infty} \int \varphi(x) \int p^{(n-1)}(x, w) P(w, A) dw dx$$

where  $p^{(n-1)}(x, w)$  is the density associated with  $P^{(n-1)}(x, \cdot)$ .

Proof (continued): Then,

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*ie*: 
$$P^{(n-1)}(x,B) = \int_B p^{(n-1)}(x,w) dw$$

Proof (continued):

$$\gamma_{\varphi}(A) = \lim_{n \to \infty} \int \varphi(x) \int p^{(n-1)}(x, w) P(w, A) \, dw \, dx$$

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Proof (continued):

$$\begin{aligned} \gamma_{\varphi}(A) &= \lim_{n \to \infty} \int \varphi(x) \int p^{(n-1)}(x, w) P(w, A) \, dw \, dx \\ &= \lim_{n \to \infty} \int \left[ \int \varphi(x) p^{(n-1)}(x, w) \, dx \right] \, P(w, A) \, dw \end{aligned}$$

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#### $\Rightarrow \gamma_{arphi}$ is stationary

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- Often the limit is independent of the starting distribution.

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 So, <u>if</u> the stationary distribution π is unique and if a limiting distribution exists, that limiting distribution <u>is</u> π:

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or

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 So, <u>if</u> the stationary distribution π is unique and if a limiting distribution exists, that limiting distribution <u>is</u> π:

$$\lim_{n \to \infty} P^{(n)}(x, A) = \pi(A)$$
$$\lim_{n \to \infty} p^{(n)}(x, y) = \pi(y)$$

or

or (discrete state space)

$$\lim_{n\to\infty}p_{ij}^{(n)}=\pi_j$$

This forms the basis for all "Markov chain Monte Carlo" (MCMC) methods.

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We either:

• have some sort of Markov process for which we want to understand an equilibrium distribution

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This forms the basis for all "Markov chain Monte Carlo" (MCMC) methods.

We either:

- have some sort of Markov process for which we want to understand an equilibrium distribution
- have a (target) distribution we want to draw from for which we will create a Markov chain that will converge in distribution towards the target distribution

A Simple Example:

Let  $\{X_n\}$  be a Markov chain on  $S = \{0, 1\}$  with probability transition matrix

 $\mathcal{P} = \left[ \begin{array}{cc} 0.99 & 0.01 \\ 0.08 & 0.92 \end{array} \right]$ 

Let's find the distribution  $\pi$ .

We need to specify  $\pi_0$  and  $\pi_1$ .

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Recall that  $\pi$  satifies

$$\pi_j = \sum_{i \in S} \pi_i p_{ij}$$

for all *j*.

In other "words":

$$\vec{\pi} = \vec{\pi} \mathcal{P}$$

where  $\vec{\pi} = (\pi_0, \pi_1, ...)$ .

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Back to the Example:

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$$\mathcal{P} = \left[ \begin{array}{cc} 0.99 & 0.01 \\ 0.08 & 0.92 \end{array} \right]$$

In this case,

$$\pi_0 = 8/9, \qquad \pi_1 = 1/9.$$

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Seeing stationarity in action:

$$\mathcal{P} = \begin{bmatrix} 0.99 & 0.01 \\ 0.08 & 0.92 \end{bmatrix} \qquad \qquad \pi_0 = 8/9, \qquad \pi_1 = 1/9$$

- I started 100,000 sample paths (realizations of  $\{X_n\}$ ).
  - with probability 8/9, I started from 0
  - with probability 1/9, I started from 1
- I ran each path for one time step according to  $\mathcal{P}$ .

Results:

- 89,012 trials resulted in 0
- 10,988 trials resulted in 1

ie:

$\hat{\pi}_{0}$	=	0.89012
$\hat{\pi}_1$	=	0.10988

Seeing limiting behavior in action:

- I started 100,000 sample paths, <u>all</u> from state 0, and ran for one time step. Results
  - 98,955 trials resulted in 0
  - 1,045 trials resulted in 1

ie: after 1 step

 $\hat{\pi}_0 = 0.98955$  $\hat{\pi}_1 = 0.01045$ 

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Repeated estimates for  $\pi_0$  for samples of size 100,000:

1 step	2 steps	3 steps
0.98955	0.98099	0.97318
0.98992	0.98104	0.97316
0.98972	0.98102	0.97247
10 steps	25 steps	100 steps
0.93196	0.89821	0.88874
0.93321	0.89855	0.88894
0.93210	0.89920	0.89009

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We could have predicted these results since a 3 step simulation, for example, is a single step simulation with transition probability matrix

$$\mathcal{P}_3 = \mathcal{P}^{(3)} = \mathcal{P}^3 = \begin{bmatrix} 0.972619 & 0.027281\\ 0.219048 & 0.780952 \end{bmatrix}$$

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The 25 step transition probability matrix is the first one to break the 0.90/0.80 barrier for  $0 \rightarrow 0$ :

$$\mathcal{P}_{25} = \mathcal{P}^{(25)} = \mathcal{P}^{25} = \begin{bmatrix} 0.8994... & 0.1006... \\ 0.8048... & 0.1952... \end{bmatrix}$$

(Still hasn't converged because the columns haven't "stabilized".)

At 50, the transitions really start to settle down,

$$\mathcal{P}_{50} = \mathcal{P}^{(50)} = \mathcal{P}^{50} = \begin{bmatrix} 0.8899...& 0.1101...\\ 0.8809...& 0.1191... \end{bmatrix}$$

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In general, the question of "How far do I need to go?" to see this convergence is a really tough question to answer and is different for each "type" of Markov chain!

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# Analysis of Convergence Rate via Eigenvalues

Stationarity:

$$\vec{\pi}\mathcal{P}=\vec{\pi}$$

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Note that  $\vec{\pi}$  is a (left) eigenvector of the transition matrix corresponding to the eigenvalue 1.

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Facts:

- The determinant of a stochastic matrix is at most 1.
- The largest eigenvalue of a stochastic matrix is 1.

(Perron-Frobenius Theorem)

We consider the case of a unique stationary distribution. (ie: only one eigenvector associated with eigenvalue 1.

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Denote all eigenvalues

 $1 = \lambda_1 > |\lambda_2| \ge |\lambda_3| \ge \cdots$ 

and associated eigenvectors

 $\pi, \vec{v}_2, \vec{v}_3, \cdots$ 

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We can represent the intial distribution

 $\vec{\varphi} = \vec{\pi} + a_2 \vec{v}_2 + a_3 \vec{v}_3 + \cdots$ 

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 $\vec{\varphi} = \vec{\pi} + a_2 \vec{v}_2 + a_3 \vec{v}_3 + \cdots$ 

Then, starting with a draw from  $\vec{\varphi}$ , the distribution of the chain after *n* steps is

 $P_{\varphi}(X_n = i) = i^{th}$  component of  $\vec{\varphi} \mathcal{P}^n$ 

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But,

$$\varphi \mathcal{P}^n = \vec{\pi} \mathcal{P}^n + a_2 \vec{v}_2 \mathcal{P}^n + a_3 \vec{v}_3 \mathcal{P}^n + \cdots$$

$$\stackrel{stat.\&evals}{=} \quad \vec{\pi} + a_2 \lambda_2^n \vec{v}_2 + a_3 \lambda_3^n \vec{v}_3 + \cdots$$

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Since the  $\lambda$ 's have magnitude smaller than 1, as *n* increases  $\varphi \mathcal{P}^n$  will converge to  $\vec{\pi}$  with a rate of convergence governed by the magnitude of the second largest eigenvalue ( $\lambda_2$ ) of  $\mathcal{P}$ .

In particular

$$||P^{(n)}(x,\cdot)-\pi||_{TV} \le C\lambda_2^n$$

where  $||\mu - \nu||_{TV}$  is the total variation norm distance defined by

$$||\mu - \nu||_{TV} = \max_{A \subseteq S} |\mu(A) - \nu(A)|.$$

One can show that if  $\mu$  and  $\nu$  are discrete densities,

$$||\mu - \nu||_{TV} = \frac{1}{2} \sum_{x \in S} |\mu(x) - \nu(x)|.$$

To explore existence and uniqueness, we need a different classification of states based on the mean recurrence time:

 $\mu_i = \mathsf{E}_i[T_i]$ 

where  $T_i = \min\{n \ge 1 : X_n = i\}$ 

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To explore existence and uniqueness, we need a different classification of states based on the mean recurrence time:

$$\mu_i = \mathsf{E}_i[T_i]$$

where  $T_i = \min\{n \ge 1 : X_n = i\}$ 

A recurrent state for a Markov chain is one that you will eventually return to with probability 1. It is

- positive recurrent if  $\mu_i < \infty$
- null recurrent if  $\mu_i = \infty$

(If there is some positive probability to get away, never to return again, the state is called transient).

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Theorem: Let  $\{X_n\}_{n\geq 0}$  be an irreducible Markov chain.

(irreducible= all states can be reached from all states)

A) If the chain has stationary distribution  $\pi$ , then  $\pi$  is given by

$$\pi(i) = \frac{1}{\mathsf{E}_i[T_i]}$$

(Hence  $\pi$  is unique!) (Moreover, all states are positive recurrent!)

#### Theorem:

B) Conversely, if the chain is positive recurrent (all states positive recurrent), then  $\pi,$  defined by

$$\pi(i) = \frac{1}{\mathsf{E}_i[T_i]}$$

is the unique stationary distribution.

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- I started 100,000 sample paths from 0
- I ran each path until 0 was hit at time n > 0
- Results:

The average number of steps it took to hit 0 starting from 0:

$$1.1251 \quad \Rightarrow \quad \hat{\pi}(0) = \frac{1}{1.1251} \approx 0.88881$$

Similarly,

- I started 100,000 sample paths from 1
- I ran each path until 1 was hit at time n > 0 item Results:

The average number of steps it took to hit 1 starting from 1:

$$8.9978 \ \Rightarrow \ \hat{\pi}(1) = rac{1}{8.9978} pprox 0.11138$$

#### Theorem:

An irreducible aperiodic Markov chain belongs to one of the following classes:

- I. All states are transient or all are null recurrent. In this case,  $\lim_{n\to\infty} P^{(n)}(i,j) = 0$  for all i,j and there is no stationary distribution.
- II. All states are positive recurrent. In this case

$$\pi_j = \lim_{n \to \infty} P^{(n)}(i,j) > 0$$

is the unique stationary distribution.