

# Markov chains

Dr. Jarad Niemi

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# Discrete-time, discrete-space Markov chain theory

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# Markov chains

## Definition

A **discrete-time, time-homogeneous Markov chain** is a sequence of random variables  $\theta^{(t)}$  such that

$$p\left(\theta^{(t)} \mid \theta^{(t-1)}, \dots, \theta^{(0)}\right) = p\left(\theta^{(t)} \mid \theta^{(t-1)}\right)$$

which is known as the **transition distribution**.

## Definition

The **state space** is the support of the Markov chain.

## Definition

The transition distribution of a Markov chain whose state space is finite can be represented with a **transition matrix**  $P$  with elements  $P_{ij}$  representing the probability of moving from state  $i$  to state  $j$  in one time-step.

# Correlated coin flip

Let

$$P = \begin{matrix} & \begin{matrix} 0 & 1 \end{matrix} \\ \begin{matrix} 0 \\ 1 \end{matrix} & \begin{pmatrix} 1-p & p \\ q & 1-q \end{pmatrix} \end{matrix}$$

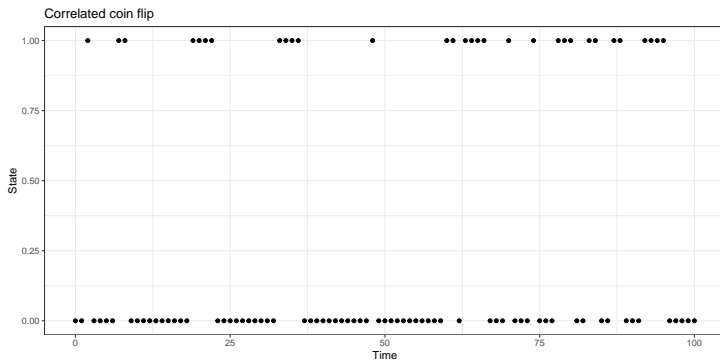
where

- the state space is  $\{0, 1\}$ ,
- $p$  is the probability of switching from 0 to 1, and
- $q$  is the probability of switching from 1 to 0.

# Correlated coin flip

$$p=0.2, q=0.4$$

Warning: 'qplot()' was deprecated in ggplot2 3.4.0.  
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Call 'lifecycle::last\_lifecycle\_warnings()' to see where this warning was generated.



# DNA sequence

$$P = \begin{array}{c} A \\ C \\ G \\ T \end{array} \begin{pmatrix} A & C & G & T \\ 0.60 & 0.10 & 0.10 & 0.20 \\ 0.10 & 0.50 & 0.30 & 0.10 \\ 0.05 & 0.20 & 0.70 & 0.05 \\ 0.40 & 0.05 & 0.05 & 0.50 \end{pmatrix}$$

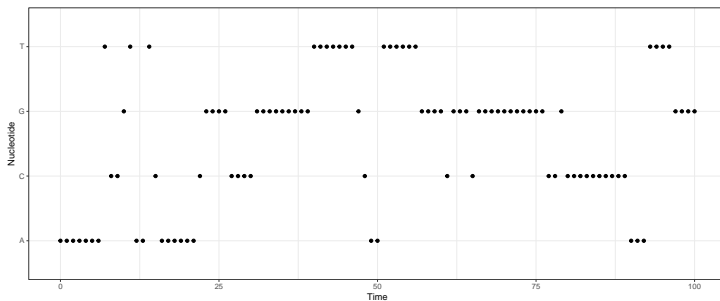
with

- state space  $\{A, C, G, T\}$  and
- each cell provides the probability of moving from the row nucleotide to the column nucleotide.

<http://tata-box-blog.blogspot.com/2012/04/introduction-to-markov-chains-and.html>

# DNA sequence

```
[1] A A A A A A A T C C G T A A T C A A A A A C G G G G C C C C G G G G G G G G T T T T T T T G C A A T T
[58] G G G G C G G G C G G G G G G G G G G C C G C C C C C C C C C A A A T T T T G G G G
Levels: A C G T
```



# Random walk on the integers

Let

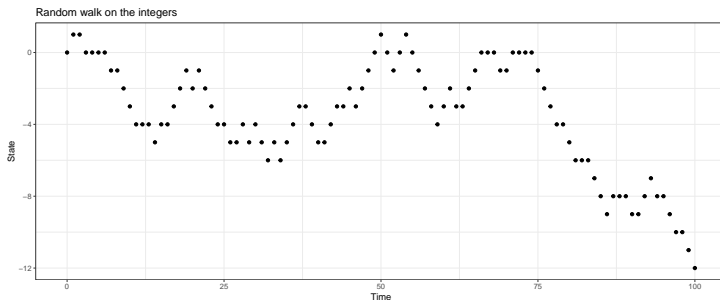
$$P_{ij} = \begin{cases} 1/3 & j \in \{i-1, i, i+1\} \\ 0 & \text{otherwise} \end{cases}$$

where

- the state space is the integers, i.e.  $\{\dots, -1, 0, 1, \dots\}$  and
- the transition matrix  $P$  is infinite-dimensional.



# Random walk on the integers



# Stationary distribution

Let  $\pi^{(t)}$  denote a row vector with

$$\pi_i^{(t)} = Pr\left(\theta^{(t)} = i\right).$$

Then

$$\pi^{(t)} = \pi^{(t-1)} P.$$

Thus,  $\pi^{(0)}$  and  $P$  completely characterize  $\pi^{(t)} = \pi^{(0)} P^t$  where  $P^t = P^{t-1} P$  for  $t > 1$  and  $P^1 = P$ .

## Definition

A **stationary distribution** is a distribution  $\pi$  such that

$$\pi = \pi P.$$

This is also called the **invariant** or **equilibrium distribution**.

Given a transition matrix  $P$ ,

- Does a  $\pi$  exist? Is  $\pi$  unique?
- If  $\pi$  is unique, does  $\lim_{t \rightarrow \infty} \pi^{(t)} = \pi$  for all  $\pi^{(0)}$ ? In this case,  $\pi$  is often called the **limiting distribution**.

# Stationary distribution exists, but is not unique

Let

$$P = \begin{matrix} & \begin{matrix} 0 & 1 \end{matrix} \\ \begin{matrix} 0 \\ 1 \end{matrix} & \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{matrix}$$

then

$$\pi = \pi P$$

for any  $\pi$ .

This Markov chain stays where it is.

# Irreducibility

## Definition

A Markov chain is **irreducible** if for all  $i$  and  $j$

$$Pr\left(\theta^{t_{ij}} = j \mid \theta^{(0)} = i\right) > 0$$

for some  $t_{ij} \geq 0$ . Otherwise the chain is **reducible**.

## Theorem

A **finite** state space, **irreducible** Markov chain has a unique stationary distribution  $\pi$ .

Reducible example:

$$P = \begin{matrix} & \begin{matrix} 0 & 1 & 2 & 3 \end{matrix} \\ \begin{matrix} 0 \\ 1 \\ 2 \\ 3 \end{matrix} & \begin{pmatrix} 0.5 & 0.5 & 0 & 0 \\ 0.5 & 0.5 & 0 & 0 \\ 0 & 0 & 0.5 & 0.5 \\ 0 & 0 & 0.5 & 0.5 \end{pmatrix} \end{matrix}$$

Stationary distribution is unique, but is not the limiting distribution.

Let

$$P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

then  $\pi = (\frac{1}{2} \ \frac{1}{2})$  since  $\pi = \pi P$ , but

$$\lim_{t \rightarrow \infty} \pi^{(t)} \neq \pi \ \forall \ \pi^{(0)}$$

since

$$\pi^{(t)} = \begin{cases} \pi^{(0)} & t \text{ even} \\ 1 - \pi^{(0)} & t \text{ odd} \end{cases}$$

This Markov chain jumps back and forth.

# Aperiodic

## Definition

The **period**  $k_i$  of a state  $i$  is

$$k_i = \gcd\{t : \Pr(\theta^{(t)} = i | \theta^{(0)} = i) > 0\}$$

where gcd is the greatest common divisor. If  $k_i = 1$ , then state  $i$  is said to be **aperiodic**, i.e.

$$\Pr(\theta^{(t)} = i | \theta^{(0)} = i) > 0$$

for  $t > t_0$  for some  $t_0$ . A Markov chain is **aperiodic** if every state is aperiodic.

Periodic example:

$$P = \begin{matrix} & \begin{matrix} 0 & 1 & 2 & 3 \end{matrix} \\ \begin{matrix} 0 \\ 1 \\ 2 \\ 3 \end{matrix} & \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix} \end{matrix}$$

# Example

Let

$$P = \begin{matrix} & \begin{matrix} 0 & 1 \end{matrix} \\ \begin{matrix} 0 \\ 1 \end{matrix} & \begin{pmatrix} 0 & 1 \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \end{matrix}$$

Note that

$$\begin{aligned} Pr(\theta^{(1)} = 0 | \theta^{(0)} = 0) &= 0 \\ Pr(\theta^{(2)} = 0 | \theta^{(0)} = 0) &= \frac{1}{2} \\ Pr(\theta^{(3)} = 0 | \theta^{(0)} = 0) &= \frac{1}{2} \frac{1}{2} = \frac{1}{4} \\ Pr(\theta^{(4)} = 0 | \theta^{(0)} = 0) &= \frac{1}{2} \frac{1}{2} + \frac{1}{2} \frac{1}{2} \frac{1}{2} = \frac{3}{8} \\ &\vdots \end{aligned}$$

generally  $Pr(\theta^{(t)} = 0 | \theta^{(0)} = 0) > 0$  for all  $t > 1$ . The **period**  $k$  of state 0 is

$$\gcd\{t : Pr(\theta^{(t)} = i | \theta^{(0)} = i) > 0\} = \gcd\{2, 3, 4, 5, \dots\} = 1$$

Thus state 0 is aperiodic. State 1 is trivially aperiodic since  $P(\theta^{(1)} = 1 | \theta^{(0)} = 1) = 1/2 > 0$ . Thus the Markov chain is aperiodic.

# Finite support convergence

## Lemma

*Every state in an irreducible Markov chain has the same period. Thus, in an irreducible Markov chain, if one state is aperiodic, then the Markov chain is aperiodic.*

## Theorem

A *finite* state space, *irreducible* Markov chain has a unique stationary distribution  $\pi$ . If the chain is *aperiodic*, then  $\lim_{t \rightarrow \infty} \pi^{(t)} = \pi$  for all  $\pi^{(0)}$ .



# Correlated coin flips

For

$$P = \begin{matrix} & \begin{matrix} 0 & 1 \end{matrix} \\ \begin{matrix} 0 \\ 1 \end{matrix} & \begin{pmatrix} 1-p & p \\ q & 1-q \end{pmatrix} \end{matrix}$$

is irreducible and aperiodic if  $0 < p, q < 1$ , thus the Markov chain with transition matrix  $P$  has a unique stationary distribution and the chain converges to this distribution.

Since  $\pi = \pi P$  and  $\pi_0 + \pi_1 = 1$ , we have

$$\begin{aligned} \pi_0 &= \pi_0(1-p) + \pi_1 q \implies \\ \frac{p}{q} &= \frac{\pi_1}{\pi_0} = \frac{\pi_1}{1-\pi_1} \implies \\ \pi_1 &= \frac{p}{p+q} \implies \\ \pi_0 &= \frac{q}{p+q} \end{aligned}$$

So, the stationary distribution for  $P$  is  $\pi = (q, p)/(p+q)$ .

# Calculate numerically

For finite state space and  $P^t = P^{t-1}P$ , we have

$$\lim_{t \rightarrow \infty} \pi^{(t)} = \lim_{t \rightarrow \infty} \pi^{(0)} P^t = \pi^{(0)} \lim_{t \rightarrow \infty} P^t = \pi^{(0)} \begin{bmatrix} \pi \\ \vdots \\ \pi \end{bmatrix} = \pi$$

```
p = 0.2; q = 0.4
create_P = function(p,q) matrix(c(1-p,p,q,1-q), 2, byrow=TRUE)
P = Pt = create_P(p,q)
for (i in 1:100) Pt = Pt**P
Pt
```

```
      [,1]      [,2]
[1,] 0.6666667 0.3333333
[2,] 0.6666667 0.3333333
```

```
c(q,p)/(p+q)
```

```
[1] 0.6666667 0.3333333
```

# Random walk on the integers

Let

$$P_{ij} = \begin{cases} 1/3 & j \in \{i-1, i, i+1\} \\ 0 & \text{otherwise} \end{cases}.$$

Then, this Markov chain is

- irreducible

$$Pr\left(\theta^{(|j-i|)} = j \mid \theta^{(0)} = i\right) = 3^{-|j-i|} > 0,$$

- and aperiodic

$$Pr\left(\theta^{(t)} = i \mid \theta^{(t-1)} = i\right) = 1/3 > 0,$$

but the Markov chain does not have a stationary distribution.

The Markov chain can wander off forever.

A stationary distribution must satisfy  $\pi = \pi P$  with

$$P = \begin{pmatrix} & & & \vdots & & & & \\ \cdots & 0 & 1/3 & 1/3 & 1/3 & 0 & 0 & 0 & \cdots \\ & 0 & 0 & 1/3 & 1/3 & 1/3 & 0 & 0 & \\ & 0 & 0 & 0 & 1/3 & 1/3 & 1/3 & 0 & \\ & & & \vdots & & & & \end{pmatrix}$$

or, more succinctly,

$$\pi_i = \frac{1}{3}\pi_{i-1} + \frac{1}{3}\pi_i + \frac{1}{3}\pi_{i+1}.$$

Thus we must solve for  $\{\pi_i\}$  that satisfy

$$\begin{aligned} 2\pi_i &= \pi_{i-1} + \pi_{i+1} \quad \forall i \\ \sum_{i=-\infty}^{\infty} \pi_i &= 1 \\ \pi_i &\geq 0 \quad \forall i \end{aligned}$$

Note that

$$\begin{aligned} \pi_2 &= 2\pi_1 - \pi_0 \\ \pi_3 &= 2\pi_2 - \pi_1 = 3\pi_1 - 2\pi_0 \\ &\vdots \\ \pi_i &= i\pi_1 - (i-1)\pi_0 \end{aligned}$$

Thus

$$\begin{aligned} \text{if } \pi_1 = \pi_0 > 0, & \quad \text{then } \pi_i = \pi_1, \forall i \geq 2 \text{ and } \sum_{i=0}^{\infty} \pi_i > 1 \\ \text{if } \pi_1 > \pi_0, & \quad \text{then } \pi_i \rightarrow \infty \\ \text{if } \pi_1 < \pi_0, & \quad \text{then } \pi_i \rightarrow -\infty \\ \text{if } \pi_1 = \pi_0 = 0, & \quad \text{then } \pi_i = 0 \quad \forall i \geq 0 \end{aligned}$$

But we also have  $\pi_i = 2\pi_{i+1} - \pi_{i+2}$  so that

$$\text{if } \pi_1 = \pi_0 = 0, \quad \text{then } \pi_i = 0 \quad \forall i \leq 0$$

Thus a stationary distribution does not exist.

# Recurrence

## Definition

Let  $T_i$  be the first return time to state  $i$ , i.e.

$$T_i = \inf\{t \geq 1 : \theta^{(t)} = i | \theta^{(0)} = i\}$$

A state is **recurrent** if  $Pr(T_i < \infty) = 1$  and is **transient** otherwise. A recurrent state is **positive recurrent** if  $E[T_i] < \infty$  and is **null recurrent** otherwise. A Markov chain is called **positive recurrent** if all of its states are positive recurrent.

## Lemma

*If a Markov chain is irreducible and one of its states is positive (null) recurrent, then all of its states are positive (null) recurrent.*

## Lemma

*If state  $i$  of a Markov chain is aperiodic, then  $\lim_{t \rightarrow \infty} \pi_i^{(t)} = 1/E[T_i]$ .*

# Ergodic theorem

## Theorem

For an *irreducible* and *aperiodic* Markov chain,

- if the Markov chain is *positive recurrent*, then there exists a unique  $\pi$  so that  $\pi = \pi P$  and  $\lim_{t \rightarrow \infty} \pi^{(t)} = \pi$  with  $\pi_i = 1/E[T_i]$ ,
- if there exists a positive vector  $\pi$  such that  $\pi = \pi P$  and  $\sum_i \pi_i = 1$ , then it must be the stationary distribution and  $\lim_{t \rightarrow \infty} \pi^{(t)} = \pi$ , and
- if there exists a positive vector  $\pi$  such that  $\pi = \pi P$  and  $\sum_i \pi_i$  is infinite, then a stationary distribution does not exist and  $\lim_{t \rightarrow \infty} \pi_i^{(t)} = 0$  for all  $i$ .

If the chain is irreducible, aperiodic, and positive recurrent, we call it *ergodic*.

When the state-space of the Markov chain has continuous support, then we talk about probabilities of being in sets, e.g.  $\pi_i = P(\theta \in A_i)$ .

# Autoregressive process of order 1

Let the transition distribution be

$$\theta^{(t)} | \theta^{(t-1)} \sim N(\mu + \rho[\theta^{(t-1)} - \mu], \sigma^2).$$

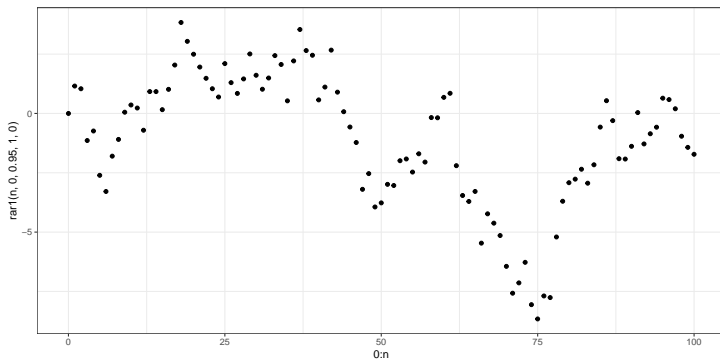
with  $|\rho| < 1$ . This defines an autoregressive process of order 1.

It is

- irreducible
- aperiodic, and
- positive recurrent.

Thus this Markov chain has a stationary distribution and converges to that stationary distribution.

# Autoregressive process of order 1





# Stationary distribution for AR1 process

Let  $\theta^{(t)} | \theta^{(t-1)} \sim N(\mu + \rho[\theta^{(t-1)} - \mu], \sigma^2)$ , or, equivalently

$$\theta^{(t)} = \mu + \rho[\theta^{(t-1)} - \mu] + \epsilon_t$$

where  $\epsilon_t \sim N(0, \sigma^2)$ . If  $\theta^{(t-1)} \sim N(\mu, \sigma^2/[1 - \rho^2])$ , then

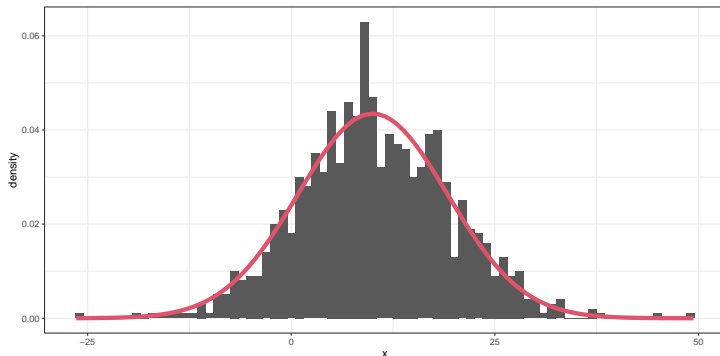
$$\begin{aligned} E[\theta^{(t)}] &= \mu \\ V[\theta^{(t)}] &= \rho^2 \frac{\sigma^2}{1 - \rho^2} + \sigma^2 = \frac{\sigma^2}{1 - \rho^2} \end{aligned}$$

Thus  $\theta^{(t)} \sim N(\mu, \sigma^2/[1 - \rho^2])$  is the stationary distribution for an AR1 process.

# Approximate via simulation

```
mu = 10; sigma = 4; rho = 0.9
```

Warning: The dot-dot notation ('..density..') was deprecated in ggplot2 3.4.0.  
Please use 'after\_stat(density)' instead.  
This warning is displayed once every 8 hours.  
Call 'lifecycle::last\_lifecycle\_warnings()' to see where this warning was generated.



# Summary

Markov chains converge to their stationary distribution if the chain is ergodic, i.e. it is

- aperiodic,
- irreducible, and
- positive recurrent

MCMC algorithms, e.g. Gibbs sampling, Metropolis-Hastings, and Metropolis-within-Gibbs, by construction

- have a unique stationary distribution  $p(\theta|y)$  and
- converge to that stationary distribution.