

## Absorbing Markov chains (sections 11.1 and 11.2)

What is a Markov chain, really?

That is, what kind of mathematical object is it?

It's NOT a special kind of stochastic matrix (although we do use stochastic matrices to understand the behavior of Markov chains).

An  $n$ -state Markov chain is a probability measure on a space of (finite or infinite) sequences of states.

It's easiest to explain this in the case of an absorbing Markov chain.

Example: The Markov chain on the state-space  $\{1,2,3,4\}$  with transition matrix

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

and initial state 2 is a random variable taking the value  $(2,1,1,1,1,1,\dots)$  with probability

$$p_{21} p_{11} p_{11} p_{11} p_{11} \dots = 1/2,$$

the value  $(2,3,4,4,4,4,\dots)$  with probability

$$p_{23} p_{34} p_{34} p_{34} p_{34} \dots = 1/4,$$

the value  $(2,3,2,1,1,1,\dots)$  with probability

$$p_{23} p_{32} p_{21} p_{11} p_{11} \dots = 1/8,$$

the value  $(2,3,2,3,4,4,\dots)$  with probability

$$p_{23} p_{32} p_{23} p_{34} p_{44} \dots = 1/16,$$

et c.

(and all other values have probability 0).

Note that (using the terminology introduced in the second lecture), things like  $(2,3,4,4,4,4,\dots)$  are not "states" but out comes, or elements of the probability space.

We have an (infinite) probability space

$$\Omega = \{\omega_1, \omega_2, \omega_3, \omega_4, \dots\}$$

with

$$\omega_1 = (2, 1, 1, 1, 1, 1, \dots),$$

$$\omega_2 = (2, 3, 4, 4, 4, 4, \dots),$$

$$\omega_3 = (2, 3, 2, 1, 1, 1, \dots),$$

$$\omega_4 = (2, 3, 2, 3, 4, 4, \dots),$$

...

and a probability measure  $m$  satisfying

$$m(\omega_i) = 1/2^i \text{ for all } i.$$

If you want, you can include the outcome  $(2, 3, 2, 3, 2, 3, \dots)$ , which has probability 0.

Or you can leave it out. Either way, we get a set of outcomes, and an assignment of probabilities to those outcomes such that every outcome has non-negative probability and the sum of the probabilities of all the outcomes equals 1, which is precisely what we mean by a probability space.

Sometimes it's more handy to index time starting from 0 rather than 1; that is, we use  $(x_0, x_1, x_2, \dots)$  instead of  $(x_1, x_2, x_3, \dots)$ .

We formalize the notion of an  $n$ -state Markov chain by defining the set

$$\Omega = \{(x_0, x_1, x_2, \dots): 1 \leq x_i \leq n \text{ for all } i \geq 0\}$$

and turning it into the probability space by giving it the probability measure

$$m((x_0, x_1, x_2, \dots)) = q_{x_0} p_{x_0 x_1} p_{x_1 x_2} p_{x_2 x_3} \dots$$

This prescription for building a probability space doesn't make sense for all Markov chains; e.g., if  $\mathbf{P}$  is the 2-by-2 matrix

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

then for every  $(x_0, x_1, x_2, \dots)$  we get an infinite product with infinitely many factors equal to  $1/2$ , which converges to 0. So each individual outcome  $\omega$  has  $m(\omega) = 0$ ! Later on I'll say a little bit about how we make sense of Markov chains in such cases.

But for absorbing Markov chains, it turns out we don't

have to worry about such things.

**Fact:** If the Markov chain associated with the matrix  $\mathbf{P}$  is absorbing, then the sum of  $m(\omega)$  over all  $\omega$  in  $\Omega$  is 1. So we have a well-defined discrete probability space. (Note: For some sequences  $\omega$  we have  $m(\omega) = 0$  because one of the transitions in  $\omega$  corresponds to an entry of the transition matrix that equals 0.

E.g., for our standard 4-state example,  $m((2,3,2,2,1,1,1,\dots))$  because  $p_{22} = 0$ .

And for other sequences  $\omega$  we have  $m(\omega) = 0$  because the infinite product vanishes, even if none of the factors vanish.

E.g., for our standard 4-state example,  $m((2,3,2,3,2,3,\dots)) = (1/2)(1/2)(1/2)\dots = 0$ .

But because every absorbing Markov chain has states  $x$  with  $p_{xx} = 1$ , we have many outcomes  $\omega$  with  $m(\omega) > 0$ .

And indeed if we sum  $m(\omega)$  over all  $\omega$  we get 1, as long as our Markov chain is an absorbing Markov chain.

This means that to compute the probability of some event  $E \subseteq \Omega$  we just need to compute the (possibly infinite) sum  $\sum_{\omega \in E} m(\omega)$ .

E.g., returning to our favorite example, to compute the probability of the event "The Markov chain eventually gets to state 4", we compute  $\text{Prob}(\{\omega_2, \omega_4, \dots\}) = m(\omega_2) + m(\omega_4) + \dots = 1/4 + 1/16 + \dots = 1/3$ .

For most absorbing Markov chains, the space of outcomes has a much more complicated structure, so we can't answer questions like this by just summing geometric series. Instead, we use linear algebra.

For instance, returning to our favorite 4-state Markov chain, the probability the chain enters state 4 within

10 steps can be computed as the 2,4th entry of the matrix  $\mathbf{P}^{10}$ , and the probability that the chain eventually enters state 4 can be computed as the 2,4th entry of the matrix

$$\mathbf{P}^\infty := \lim_{n \rightarrow \infty} \mathbf{P}^n.$$

*Mathematica* caveat: don't confuse  $\mathbf{P}^n$  with `MatrixPower[P,n]`!:

```
P = {{1, 0, 0, 0}, {1/2, 0, 1/2, 0}, {0, 1/2, 0, 1/2}, {0, 0, 0, 1}}
```

```
P^2
```

```
MatrixPower[P, 2]
```

```
N[MatrixPower[P, 10][[2, 4]]]
```

```
Limit[MatrixPower[P, m], m -> Infinity][[2, 4]]
```

But don't make the mistake of confusing these kinds of calculations with simulations, and don't mistake a Markov chain (a probability distribution on sequences of states) with the associated matrix.

The matrix

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

is just a matrix, not a Markov chain; its entries determine a probability measure on the space of sequences of 1's, 2's, 3's and 4's, and this probability measure is what we mean by a Markov chain.

More generally, a probability space whose outcomes are sequences is called a **discrete-time stochastic process**.

(Note that a sequence  $\omega = (x_0, x_1, x_2, \dots)$  can also be thought of as a function whose domain is the set of non-negative integers. Later we'll see probability spaces whose outcomes are functions on  $\{t \in \mathbb{R}: t \geq 0\}$  rather than on  $\{0, 1, 2, \dots\}$ ; such a probability space is called a **continuous-time stochastic process**.)

When the elements of  $\Omega$  are sequences of the form  $(x_0, x_1, x_2, \dots)$  (where  $x_0, x_1, x_2, \dots$  are elements of  $\{1, 2, 3, \dots, n\}$ ), it's natural to define random variables  $X_0, X_1, X_2, \dots$  on  $\Omega$ . Remember that a random variable is just a function on  $\Omega$ . We define

$$X_0(x_0, x_1, x_2, \dots) = x_0,$$

$$X_1(x_0, x_1, x_2, \dots) = x_1,$$



$$X_2(x_0, x_1, x_2, \dots) = x_2,$$

etc.

So a random element of  $\Omega$  can (somewhat circularly!) be written as the sequence

$$(X_0(\omega), X_1(\omega), X_2(\omega), \dots)$$

Note that we've been taking the  $x$ 's to be elements of  $\{1, 2, \dots, n\}$  where  $n$  is the number of states. This is a good choice when the states ARE just the numbers  $1, 2, \dots, n$ ; but when the state  $s_i$  is different from the number  $i$ , it's often handy to use  $(s_{x_0}, s_{x_1}, s_{x_2}, \dots)$  instead of  $(x_0, x_1, x_2, \dots)$ .

Simulating a generic absorbing Markov chain

Simulating a Markov chain means generating a particular sequence  $x_1, x_2, x_3, \dots$  in accordance with the transition probabilities  $p_{ij}$ . More specifically, suppose you've already picked  $x_1, x_2, \dots, x_m$ , and you chose  $x_m = i$ , and now it's time to choose  $x_{m+1}$ . Then your selection procedure must have the property that your chance of choosing  $x_{m+1} = j$  should be  $p_{ij}$ , regardless of what  $x_1, x_2, \dots, x_{m-1}$  were.

That is, the probability of the compound event

$$X_1 = x_1, X_2 = x_2, X_3 = x_3, \dots, X_m = x_m$$

should be of the form

$$q_{x_1} p_{x_1 x_2} p_{x_2 x_3} p_{x_3 x_4} \dots p_{x_{m-1} x_m}$$

where  $q_{x_1}$  is the probability  $\text{Prob}(X_1 = x_1)$ .

Let's write code to simulate one step of the Markov chain associated with an  $n$ -by- $n$  transition matrix  $\mathbf{P}$ , starting from state  $i$ .

First let's solve the sub-problem of simulating a discrete random variable that takes its values on the set  $\{1, 2, \dots, n\}$ , so that the probabilities of the outcomes  $1, 2, \dots, n$  are precisely the entries of a specified probability vector  $\mathbf{v}$ .

To do this, we divide the interval  $[0, 1]$  from left to right into subintervals of lengths  $v_1, v_2, v_3, \dots$  and pick a random real number  $r$  in  $[0, 1]$ ; our output should be the unique  $i$  such that  $r$  is in  $v_i$ . Note that the subintervals are

$[0, v_1], [v_1, v_1 + v_2], [v_1 + v_2, v_1 + v_2 + v_3], \dots$ , so we can also describe the output as the smallest  $i$  such that  $v_1 + v_2 + \dots + v_i$  exceeds  $r$ .

```

DRV[v_] := (* sample from the discrete random variable associated with the vector v *)
Module[{i, sum, r},
  r = RandomReal[]; i = 1; sum = v[[1]];
  While[sum < r, i++; sum += v[[i]];
  Return[i]]
(* If we wanted more efficiency,
we could use a bisection method to find the smallest such i. *)

Table[DRV[{1/2, 1/4, 1/4}], {n, 1, 100}]

Tally[%]

Tally[Table[DRV[{1/2, 1/4, 1/4}], {n, 1, 1000}]]

```

Now it's easy to write code to simulate a single step of the Markov chain with transition matrix  $\mathbf{P}$ , starting from state  $i$ .

```
MarkovStep[P_, i_] := DRV[P[[i]]]
```

Using this we can simulate  $n$  steps of the Markov chain:

```

MarkovMultiStep[P_, i_, n_] := Module[{State = i, k},
  Print[State];
  For[k = 1, k ≤ n, k++,
    State = MarkovStep[P, State];
    Print[State]]]

(* Note that ";" takes precedence over "," in For[...] and If[...] statements! *)

P = {{1, 0, 0, 0}, {1/2, 0, 1/2, 0}, {0, 1/2, 0, 1/2}, {0, 0, 0, 1}}

MarkovMultiStep[P, 2, 10]

```

Now let's write code to simulate the chain starting from state until it enters a transient state.

```

MarkovAbsorb[P_, i_] := Module[{State = i, k},
  Print[State];
  For[k = 0, P[[State, State]] < 1, k++,
    State = MarkovStep[P, State];
    Print[State]]; Return[k]]

MarkovAbsorb[P, 2]

MarkovAbsorb[P_, i_] := Module[{State = i, k},
  For[k = 0, P[[State, State]] < 1, k++,
    State = MarkovStep[P, State]]; Return[k]]

```

Let's see what sorts of things we get if we run this process 1000 times.

```
Histogram[Table[MarkovAbsorb[P, 2], {n, 1, 1000}]]
```

For comparison, let's see what sorts of things we get if we sample from a geometric random variable (with parameter  $p = 1/2$ ) 1000 times:

```
Histogram[Table[RandomInteger[GeometricDistribution[1/2]], {n, 1, 1000}]]
```

The histograms look similar, which makes sense, because the time it takes to get from state 2 to an absorbing state is a geometric random variable with parameter  $p = 1/2$ :

Canonical form (review)

We renumber the states so that the transient states come first.

Suppose the chain has  $t$  transient states and  $r$  absorbing states. Then we can write the canonical matrix in block-form as

$$\begin{pmatrix} \mathbf{Q} & \mathbf{R} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}$$

where

$\mathbf{Q}$  is a  $t$ -by- $t$  square matrix,

$\mathbf{R}$  is a non-zero  $t$ -by- $r$  matrix,

$\mathbf{0}$  is the all-zeroes  $r$ -by- $t$  matrix, and

$\mathbf{I}$  is the  $r$ -by- $r$  identity matrix.

We say such a transition matrix is in canonical form.

Number of visits and the fundamental matrix (review)

The matrix  $\mathbf{I} - \mathbf{Q}$  is invertible (where  $\mathbf{I}$  here stands for the  $t$ -by- $t$  identity matrix), and its inverse can be written as the convergent infinite sum  $\mathbf{N} = \mathbf{I} + \mathbf{Q} + \mathbf{Q}^2 + \dots$ .

The matrix  $\mathbf{N}$  is called the fundamental matrix for the absorbing Markov chain.

Claim: The  $ij$ -entry  $n_{ij}$  of the matrix  $\mathbf{N}$  is the expected number of times the chain is in state  $s_j$ , given that it starts in state  $s_i$ . The initial state is counted (as part of "the number of times...") if  $i = j$ .

Claim: Let  $t_i$  be the expected number of steps before the chain is absorbed, given that the chain starts in state  $s_i$ , and let  $\mathbf{t}$  be the column vector whose  $i$ th entry is  $t_i$ . Then  $\mathbf{t} = \mathbf{N}\mathbf{c}$ , where  $\mathbf{c}$  is the column vector all of whose entries are 1.

Absorption probabilities

Let  $\mathbf{B} = \mathbf{N}\mathbf{R}$  (with  $\mathbf{N}, \mathbf{R}$  as in the canonical form).

Claim: The  $ij$ -entry  $b_{ij}$  of the matrix  $\mathbf{B}$  is the probability that an absorbing chain started in the transient state  $s_i$  will be absorbed in the absorbing state  $s_j$ .

Proof 1: The probability in question is equal to

$\sum_{n \geq 0} \sum_k q_{ik}^{(n)} r_{kj} = \sum_k \sum_{n \geq 0} q_{ik}^{(n)} r_{kj} = \sum_k n_{ik} r_{kj}$ , which is  $b_{ij}$ . (Here  $n$  denotes the number of steps the Markov

chain takes before it leaves the set of transient states, and  $k$  denotes the last transient state the chain visits.)

before it hits the absorbing state  $i$ , and  $n$  denotes the number of steps the chain takes

Proof 2: Let  $c_{ij}$  be the probability that an absorbing chain started in the transient state  $s_i$  will be absorbed in the absorbing state  $s_j$ . If we compute  $c_{ij}$  in terms of the possibilities on the outcome of the first step, we have

$$c_{ij} = p_{ij} + \sum_k p_{ik} c_{kj} ,$$

where  $k$  ranges over all the transient states. This is true for all  $i, j$ . This family of equations is equivalent to the single matrix equation  $\mathbf{C} = \mathbf{R} + \mathbf{Q}\mathbf{C}$ , which we can successively rewrite as  $\mathbf{C} - \mathbf{Q}\mathbf{C} = \mathbf{R}$ ,  $(\mathbf{I} - \mathbf{Q})\mathbf{C} = \mathbf{R}$ , and  $\mathbf{C} = (\mathbf{I} - \mathbf{Q})^{-1} \mathbf{R} = \mathbf{N}\mathbf{R} = \mathbf{B}$ .

`MatrixForm[FM.R]`

This agrees with what we proved before ( $P = 1/3$ ).

## Questions about the homework?

Hint for A:

See the discussion "Can we construct a Geometric( $p$ ) random variable from a Uniform(0,1) random variable?" from near the end of Lecture 2.

Hint for B:

```
P = {{.5, .5, 0}, {.25, .5, .25}, {0, .5, .5}}
N[MatrixPower[P, 1000000000]]
Limit[MatrixPower[P, k], k -> ∞]
(* What's going on here? *)
P = {{1/2, 1/2, 0}, {1/4, 1/2, 1/4}, {0, 1/2, 1/2}}
(* Moral: Don't trust Mathematica's built-
in ideas about handling limits in conjunction with decimal constants! *)
```

## ***Mathematica* reimbursement**

Please hand in your Expense Approval forms (for purchase of copies of *Mathematica*). Next Tuesday will be your last chance to do this if you want to be reimbursed anytime soon.



Name of Person or Business To Be Reimbursed: *<your name>*

Date: *<today's date>*

Department: Mathematical Sciences

Remit To Address: *<your address>*

Purpose for Incurring the Expense: Purchase of software related to PI's research

Total: [make entries on separate lines for purchase price, sales tax, and total]

Signature (Person Incurring Expense): *<your signature>*

## **Ergodic Markov chains (sections 11.3 and 11.5)**

Ergodicity

Definition 11.4: A Markov chain is called an ergodic chain if it is possible to go from every state to every state in a finite number of steps. (Note that no absorb-

ing Markov chain is ergodic, aside from the trivial absorbing Markov chains with zero or one absorbing states and no transient states.)

Example: Random walk on  $\{1,2,3,4\}$  with reflection on the ends ( $1 \rightarrow 2$  with probability  $\frac{1}{2}$  and  $4 \rightarrow 3$  with probability  $\frac{1}{2}$ ) is ergodic.

```
Ref = {{0, 1, 0, 0}, {1/2, 0, 1/2, 0}, {0, 1/2, 0, 1/2}, {0, 0, 1, 0}};
MatrixForm[MatrixPower[Ref, 4]]
```

Note that for this example, it is possible to go from every state  $s_i$  to every state  $s_j$  in a finite number  $N(i,j)$  of steps, but it is impossible to remove the dependence of  $N(i,j)$  on  $i$  and  $j$ ; that is, there does not exist  $N$  such that for all  $i$  and  $j$ , it is possible to go from  $s_i$  to  $s_j$  in exactly  $N$  steps. That is because  $N(i,j)$  must have the same parity as  $i-j$ .

We say a Markov chain is regular if there exists an  $N$  such that for all  $i$  and  $j$ , it is possible to go from  $s_i$  to  $s_j$  in exactly  $N$  steps; that is, the  $N$ th power of the transition matrix  $\mathbf{P}$  has all its entries positive (see Definition 11.5). Note that every regular Markov chain is ergodic.

The reflecting random walk described above is ergodic but not regular. A slightly different reflecting random walk that is regular can be obtained from our non-regular example by changing the behavior at the ends so that reflection is only partial:

```
ParRef = {{1/2, 1/2, 0, 0}, {1/2, 0, 1/2, 0}, {0, 1/2, 0, 1/2}, {0, 0, 1/2, 1/2}};
MatrixForm[MatrixPower[ParRef, 3]]
```